Novel precision control techniques in a trapped Yb$^+$ ion implementation

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Abstract

Precise control of quantum systems is vital to scientific and technological progress, including the realisation of quantum computation and simulation, record-breaking timekeeping and positioning applications. Control of quantum systems is hampered by the effects of random environmental or hardware noise, which leads to unknown deviations from the system’s desired evolution. This thesis presents a set of interaction-focussed methods for improving precision control, tailored to the problems of quantum error suppression and stabilisation of oscillators, which share a common basic structure. These methods are based on a theoretical framework called the filter-transfer function formalism, which expresses the convolution of user-applied control and random noise in the language of spectral filtering. This powerful and accessible approach is experimentally verified in this thesis, and is used to formulate novel control techniques and improve on existing ones. This thesis experimentally demonstrates the effectiveness of novel composite pulse schemes for suppressing error in quantum bits. Furthermore, the thesis derives and demonstrates a novel predictive technique for stabilising oscillators by means of combining multiple frequency measurements against a quantum reference. The thesis therefore advances the theoretical understanding of a frequency-domain formalism for noise-affected quantum systems, on which basis it presents and demonstrates novel and improved techniques for mitigating the effects of such noise on the user’s precision control over the system.
Statement of Contribution

I wrote this thesis. The conception, argumentation, wording and appearance of the thesis is my work and responsibility. I played a leading role in the theoretical and experimental work concerning frequency standards, presented in Chapters 6 and 7. On the qubit control project, I took the data comparing traditional composite pulses to uncompensated pulses, as well as developing the single-tone scanning technique for obtaining spectral information about an arbitrary control operation. My description of the experimental setup in Chapter 2 is based on my own laboratory notes, communication with my colleagues, precedents in the literature and equipment manuals provided by the various manufacturers. The mathematical derivations and proofs presented in Chapter 3 are my own synthesis of the existing literature.

What I have presented in this thesis has also relied on the work of my colleagues. Associate Professor Michael Biercuk guided and directed this project. He charted the main courses of the research of which this thesis is part, including the development of a filter function approach to universal qubit noise, the noise engineering techniques used for both experiments, and the predictive scheme for stabilising oscillators. His close oversight of the drafting of this thesis has given it a narrative consistency and a crafted purpose that would have been impossible to achieve otherwise.

MC Jarratt contributed to the optical setup for these experiments. She built the RF circuitry to drive the electro-optical modulators (EOM) at the required frequencies to produce sidebands on the laser beams, as well as writing software for a control panel to easily manipulate these frequencies. The laser frequency stabilisation setup in its current form, including the free-space UV switch driven by a custom circuit that consists of three flip-flop elements, was built by her.

Alexander Soare played a central role in building the microwave delivery system, writing the IGOR Pro software modules for coordinating the ion trap hardware and the qubit control experiment, developing the noise engineering platform using IQ modulation, as well as contributing to the optical setup. He built an early version of the laser frequency stabilisation setup using a UV switch driven by a single flip-flop element. The design and results of the qubit control experiment, in particular, owe a great debt to his involvement.

Harrison Ball did much of the legwork for the theoretical aspects of this thesis, as well as playing a leading role in conceiving of the qubit control experiment. He contributed to the development of the fidelity metric for qubit coherence and the tricky task of establishing the fit between theoretical prediction and experimental data. He played a principal role in the analysis of composite pulse schemes and comprehending them within the Walsh basis framework.

Todd Green laid the theoretical groundwork for the general approach taken in this thesis. His work on generalising the filter function to universal noise provided the mathematical tools needed to build these novel techniques for quantum control. Cody Jones worked with me on the frequency standard project in its earliest days, and wrote some important derivations for the predictive approach. Stephen Dona collected several crucial pieces of data for presentation in this thesis, assisted by Nitin Nand. David Hayes, James McLoughlin and Xinglong Zhen were involved in conceiving and building the qubit control experiment and in collecting the data for it.

Parts of the work presented here have been published or submitted elsewhere, as the products of my group’s collective research effort. Content pertaining to the qubit control experiment appeared in the Nature Physics publication [69] reproduced in Appendix A, and content pertaining to the noise
engineering technique developed by the group appeared in the *Physical Review A* publication [70] reproduced in Appendix B. I am a co-author on both of these publications and my specific contributions are indicated in each of them.

Content pertaining to the frequency standard experiment appears in two submitted works of which I am the lead author. The concept and definition of a predictive correction for oscillator stabilisation appears in my Honours thesis (submitted October 2013). More advanced stages of this work, including numerical simulations of a frequency standard undergoing predictive correction, appears a manuscript submitted to *Physical Review Letters* which is on the pre-print server [68] and is reproduced in Appendix C.

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Mike's guidance and engagement with my scientific work has been extremely dedicated. His hands-on involvement in all the projects has been most valuable to my understanding of them. His experience and knowledge of every part of the experimental apparatus has allowed me to rapidly become familiar and comfortable in using it, while his teaching of the theoretical foundations of this work has been exceptionally clear and accessible. His passion for physics and his desire to contribute to the scientific community have made for a rewarding three years for me. I thank him for the opportunities he has given me, and for his support in the conclusion of my work, which culminates in this thesis.

MC is my dearest friend in physics. She mentored me as I first learned how to work in the lab, with patience and good humour. Her sharp instinct for troubleshooting and the rigour of her experimental technique set an example that I admired and strove to follow. Her presence in the lab eased the most difficult tasks and made fun the most tedious days. Her trust and companionship have been immensely important to me, and I would be glad to have had anywhere near as positive an impact on her as she has had on me.

Alex has a breathtaking understanding of the experimental design and its operation. I relied on him a great deal to teach me how to run, fix and design the experiments described in this thesis. His ability to communicate his experience and his memory for detail were indispensable; without them I would not have been able to so quickly acquire the knowledge and skills needed to run these experiments. I have no doubt that he will establish himself as an authority in anything he turns his attention to.

Harrison has been a steadfast and dependable source of advice and solidarity. His disciplined attitude to work and commitment to thoroughness has impressed me greatly. He helped me through the challenges of theoretical physics and of working as a physicist. I wish him every good fortune for the rest of his studies and hope that they will serve him well.

Terry McRae’s humour and clear-eyed view on life has buoyed me during difficult periods, and is deeply appreciated. Based their long ion-trapping experiences, Karsten Pyka and James McLoughlin gave me advice and filled in gaps in my knowledge, thereby significantly improving my understanding.
of my work. I thank Claire Edmunds for her friendship and for helping me to complete the description of the experimental setup that appears here.

Our collaborators in South Africa, Hermann Uys and Ismail Akhalwaya, gave me many useful insights into the field. Their work, which complements my own, has enriched my understanding of the possibilities and relevance of what I have presented here. Peter Fisk and Bruce Warrington, who now lead the National Measurement Institute, once ran the ion trap that is used in these experiments. I was most grateful to have the opportunity not only to discuss with them the technical details and history of the trap, but also to seek their expert opinions on the techniques I have developed to improve oscillator stability. David Reilly and Stephen Bartlett gave me important advice and support in my degree, which I very much appreciate.

Of the many friends who have lent me a sympathetic ear, I would like to single out Steph, Eromanga and Clare, for their kindness and understanding.

Veronica has witnessed the side-effects of the tough aspects of physicist life. I thank her for her perseverance and dedication to taking care of me when I needed it, assuring me when I was concerned and calming me down when I was anxious. Her love and care have been vitalising.

Harmy’s wisdom and depth of experience have been crucial. Many moments of uncertainty and worry were resolved by her clear thinking. My written expression owes much to her careful reading, and my enthusiasm persists in no small part thanks to her encouragement.

My mum and dad gave me everything I needed to do this. At every point they have helped me to take control of events and work towards the best outcomes. Without them always behind me, of course, this thesis would be impossible.
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Chapter 1

Introduction

1.1 Introduction to precision quantum control

The ability to precisely control quantum systems is a vital requirement for the advancement of science and technology. Improvements in humans’ power to control the behaviour of quantum systems offer concrete benefits to physics and engineering communities. Speaking about atomic clocks, which are the highest-precision quantum devices in existence [8], Nobel Laureate David Wineland states that throughout history ”when a better clock was built, use was immediately found for it” [1]. High-precision control of individual quantum systems is the basis on which quantum computing may be realised [58], is necessary for quantum simulation [13] and is central to time-keeping and positioning applications [3, 48, 40]. Precision control is also necessary for fundamental science: advances in the precision of frequency standards beyond the $10^{-19}$ level could allow for laboratory-scale tests of general relativity [12] and improved bounds on the measurement of the time-variation of the fine structure constant, an empirical parameter in the Standard Model [7].

Improvement in precision control over quantum systems is, to a large extent, achieved by suppressing inaccuracies and instabilities, generically labelled as ‘error’, that result from physical noise processes. A fruitful area of research to achieve such improvements is quantum control theory, which focusses user-end techniques in order to make quantum systems more resistant to the effects of noise. The precision and stability of a quantum device, such as a quantum memory [42], may be improved by tailored error-suppressing operations performed by the experimentalist, without the need for further hardware modifications. The application of such interaction-focussed techniques to quantum systems has become prominent only since the early 2000s [77, 46], and there remains much scope for the investigation of experimentally-useful control techniques for improving the precision of realistic quantum devices, such as quantum information processors and atomic clocks [69, 68].

This thesis makes theoretical and experimental contributions to the field of precision control of quantum systems. The theoretical contributions involve the development of a unifying mathematical formalism, known as the ‘filter transfer function’ formalism, to describe the spectral response of a quantum system to an arbitrary control protocol. This formalism allows for straightforward and accurate prediction of the system’s dynamics, by capturing the sensitivity of the system to environmental and control noise. The thesis provides a comprehensive treatment of the filter transfer function formalism. On the basis of this formalism, it generalises and improves upon existing techniques for error suppression.

The experimental contributions of this thesis are: (i) the validation of the accuracy of the filter function approach in real physical systems, (ii) the development of a method for engineering artificial noise that allows the experimental apparatus to emulate a broad range of realistic noise scenarios, and (iii) demonstrating a novel predictive stabilisation scheme for oscillators that may have applications in the improvement of frequency standards, as well as general predictive control methods for sup-
pressing decoherence in quantum systems. The experimental results demonstrate the usefulness of the theory and provide a platform for optimising error-suppression protocols for other physical systems. Therefore the relevance of these results is not limited only to a particular quantum system, e.g. trapped ions, but may have direct implications for any quantum system in which precision control is a priority.

This introductory chapter is organised as follows. In Section 1.2, an explanation of precision quantum control is presented in general terms, which forms the common basis for a unified treatment of the two control problems examined in this thesis. The usefulness of a unified theoretical formalism and experimental platform is discussed. In Section 1.3 the specific features of the two control problems are introduced, to show how they focus on different parts of the same composite system. Section 1.4 is a description of the contributions made by the thesis to the scientific community, while in section 1.5 the structure of the whole thesis is outlined.

1.2 Unified approach to precision quantum control

1.2.1 Abstract features of precision control

This general description presents a unified treatment of two precision control problems that share an underlying commonality: (i) maintaining the coherence of a quantum state (the ‘quantum bit control’ problem), and (ii) stabilising the frequency of an oscillator for use as a standard (the ‘frequency standard’ problem). The two problems are associated with distinct research communities and traditions, though there has been recognition of their similarities [19]. This thesis treats the quantum bit (‘qubit’) control and frequency standard problems as having a common basic structure, showing how the same theoretical formalism (the filter transfer function approach) and the same experimental apparatus (microwave-driven trapped ions) may be used to find insights into both.

In abstract terms, the precision quantum control problems considered in this thesis involve random deviations over time from the system’s desired behaviour (‘error’), caused by instabilities in the hardware or coupling to fluctuating parameters of the environment (‘noise’). The archetypal system of interest is a two-energy-level quantum system (the quantum bit) driven by an oscillator, e.g. an atomic transition in an ion being driven by a coherent microwave source [20]. The primary source of error in the systems of interest to this thesis are fluctuations in time; spatial inhomogeneities across ensemble systems, such as are familiar from nuclear magnetic resonance (NMR) spectroscopy, are not directly targeted by the techniques developed in this thesis, although it can be shown that these techniques indirectly suppress error due to quasistatic spatial inhomogeneities.

In order to accurately control the quantum system’s behaviour, an experimentalist may use a hardware approach that involves isolating the system from environmental perturbations (e.g. shielding against magnetic field fluctuations), as well as optimising the performance of the driving oscillator. Nevertheless, improving the hardware alone is insufficient for many applications. This fact has lead to the development of interaction-focussed approaches that suppress the effects of noise by manipulating the system in such a way that the noise is cancelled. Both the controller (e.g. an oscillator) and the system (e.g. atomic transition) are susceptible to error caused by noise. An interaction-focussed approach to error-suppression involves the experimentalist modifying only the controller-system interaction, in order to make the combined setup more robust against noise. By contrast, a hardware-only approach would involve improving the controller and system individually to reduce their sensitivity to noise.

The qubit control problem and the frequency standard problem share a fundamental physical similarity. The basic architecture of both problems, which consists of a driving oscillator coupled to a quantum system, motivates a unified treatment of characterisation and methods for suppressing the effects of noise. The specific noise processes present in both cases lead to the same kinds of error in the qubit; e.g. both dephasing noise acting on a qubit from the environment and frequency noise in a local oscillator that interrogates that qubit produce the same undesired phase evolution. The type
of noise studied in this thesis is semiclassical, meaning that it produces unitary randomisation of the quantum state, rather than e.g. entanglement of the quantum system with the environment.

1.2.2 Theoretical and experimental methods

The fact that the qubit control and the frequency standard problems have the same physical structure means that the same theoretical and experimental platforms may be used to investigate them. In line with classical control theory approaches to suppressing random noise processes, the theoretical framework used in this thesis is a frequency-domain, statistical framework. The noise affecting the controller and/or system is characterised in terms of its frequency-domain power spectral density, while the action of the control protocol is quantified as a ‘filter transfer function’, also in the frequency domain. The use of frequency-domain analysis emerged independently in the quantum control [54, 47, 76] and frequency standard [14, 2, 66] communities. This thesis recognises that the same mathematics underpins both approaches, and thus develops a unified theoretical formalism in Chapter 3.

The same experimental setup is used to realise these two control problems. A high-quality oscillator that performs coherent driving on a qubit may be used either as a qubit control setup or as a frequency standard, depending on which element is used to stabilise the other. The typical quantum control experiment involves a qubit, undergoing noisy evolution due to the ambient environment, that is subjected to an open-loop control protocol by a ‘clean’ oscillator, which cancels the noise to some extent and thereby improves the experimentalist’s precision control over the qubit state. Conversely, the typical frequency standard involves an oscillator, whose frequency fluctuates randomly, being locked in a closed feedback loop to match the stable measured frequency of a qubit.

A key benefit offered by the physical commonality of the two problems is that noise in one of the elements may be used to emulate noise in the other. The noise processes in the two cases produce identical physical effects: dephasing noise in the qubit produces the same phase randomisation as frequency noise in the oscillator, while amplitude noise in the oscillator mimics the effect of relaxation of the qubit excited state. The commonality between qubit and oscillator noise allows noise to be engineered by deliberately degrading the oscillator signal according to some desired prescription [70]. If the engineered noise dominates the underlying system noise (‘intrinsic’ noise), the experimentalist may use this apparatus to emulate the kinds of noise found in other systems. The experimental apparatus used in this thesis may therefore used to test the effectiveness of various error-suppressing software protocols in a range of realistic noise scenarios.

1.3 Specifics of the control problems

1.3.1 Qubit control problem

The qubit control problem consists of a qubit that experiences noise, either due to interaction with the environment or by instabilities in the driving oscillator. The noise is described as ‘semiclassical’ because it can be modelled as a random perturbation of a classical (many-photon) field interacting with a quantum system, removing the need for a fully quantum-mechanical treatment of the oscillator-qubit interaction, e.g. that found in [76]. The primary noise mechanisms are called dephasing, which acts to randomise the relative phase between the two components of the quantum state, and driving noise, which leads to inaccuracy in the state-space trajectory of the driven quantum state during interaction with the oscillator.

The effect of such semiclassical noise is to produce ‘decoherence’ of the quantum state, which in this model refers to randomisation of the state that leads to a loss of quantum behaviour, averaged over an ensemble of identical systems [69]. So-called ‘open-loop’ techniques for mitigating the effect of noise on coherent quantum systems make use of an early insight from nuclear magnetic resonance
(NMR) spectroscopy [30], which finds that a tailored sequence of driven control operations can cancel out slowly-varying qubit noise. These techniques, which involve only the interaction between controller and system, result in a ‘recovery’ of qubit coherence at the endpoint of the sequence. The control operations therefore act as a spectral filter for the noise, since the extent of error-suppression depends on the frequency of the noise fluctuations in terms of the timescale of the control operations.

1.3.2 Frequency standard problem

The frequency standard problem consists of a ‘local oscillator’ (LO) that experiences frequency noise due to hardware instabilities or environmental perturbation. The LO frequency is compared to the characteristic frequency associated with the qubit splitting energy, which is in this problem assumed to be far more stable, by means of a spectroscopic interrogation. The resulting frequency difference information is used to correct the LO frequency in a feedback loop, thereby improving the frequency stability of the locked local oscillator (LLO). This problem belongs to the general category of ‘oscillator stabilisation’ control problems; however, due to the importance of frequency standards as the most significant example of oscillator stabilisation to a stable qubit reference, this thesis refers to this problem as the ‘frequency standard problem’.

The LO instability is quantified by metrics of variance of the measured frequency differences between the LO and qubit. The characterisation of oscillator stability is a field in its own right, with several types of variance quantity (e.g. sample variance [66], Allan variance [2], frequency variance [14, 51]) in use. The frequency standard community has developed an analytic method for calculating these variances, based on transfer functions [66]. A transfer function captures the sensitivity of its associated variance metric to the spectral content of the LO noise, thereby allowing an analytic prediction of the instability of a free-running oscillator, given spectral information about the noise and time-domain sensitivity information about the measurement sequence.

1.4 Contributions of this thesis

For the qubit control problem, this thesis seeks to develop useful methods of characterising the effect of noise on quantum coherence, and to find new control schemes with improved filtering power. In terms of characterisation methods, the thesis presents the first experimental validation of the accuracy of a filter function approach to calculating trace fidelity (a widespread metric of coherence for driven evolution). In terms of finding improved error-suppression schemes, the thesis develops a unifying theoretical framework that expresses known composite pulses in terms of the Walsh basis functions. The spectral features of these Walsh functions provide a recipe for synthesising novel composite pulse sequences with improved noise-filtering capability, hence better maintaining quantum coherence.

For the frequency standard problem, this thesis extends the transfer function method of characterising instability to apply to locked local oscillators (LLO). The contribution to characterisation involves the derivation of a recursive analytic form that may be simply expressed in the frequency domain, allowing for a direct transfer function calculation of variance for an LLO, entirely analogous to traditional calculations of LO variance. This extension to characterisation of the LLO is based on the derivation of a frequency-domain covariance function. This covariance transfer function is used, in combination with insights from optimal control theory, to develop a novel predictive technique that is presented in the thesis, which is demonstrated to improve the overall stability of the LLO. The contribution to the problem of oscillator stabilisation is the derivation and demonstration, by numerical simulation and experiment, of this predictive technique, which exploits correlations between multiple sequential measurements in order to predict the trajectory of LO noise at the moment of correction. The use of both pre-characterised spectral information and real-time measurements makes this technique a hybrid of feedback and feedforward, resulting in improved overall stability in the locked oscillator in comparison to traditional feedback methods.
1.5 Structure of thesis

The thesis is organised as follows. Chapter 2 provides a detailed description of the apparatus used to perform the experiments for the qubit control and frequency standard problems. The description includes the physics of the linear ion trap in which the experiments are conducted, the atomic physics of the ytterbium ion ensemble which constitutes the qubit, the optical system used to control and manipulate the ions, the measurement system used detect the state of the qubit and the precision microwave setup that acts as the local oscillator of the system. Particular emphasis is placed on the implementation of engineered noise to the oscillator, which is a novel technique for the emulation of quantum systems.

Chapter 3 provides theoretical background to the frequency-domain treatment of the types of semiclassical noise that are pertinent to this thesis. A rigorous definition of the power spectral density is provided for the canonical case of stochastic, Gaussian-distributed noise. The Wiener-Khinchin theorem is proven, on which the conversion from time-domain to frequency-domain calculations is based.

Chapter 4 introduces the application of the filter function formalism to universal qubit noise, via an average Hamiltonian theory. An experimentally-accessible metric for the accuracy of an arbitrary control operation, viz. the average fidelity of the operation, is derived in the convenient form of an overlap integral of the noise spectral density and the filter function.

Chapter 5 presents experimental results on the qubit control problem. The chapter verifies the accuracy of the filter function formalism in making predictions of the fidelity of qubit operations. The trapped-ion qubit is used as an experimental testing platform for the filter function approach. The usefulness of the filter function approach is further demonstrated by the improved error-suppression performance of composite pulses, as predicted by the features of their respective filter functions. The relationship between the shape of the filter function and the manner in which the pulses are synthesised in the Walsh basis allows for the search and experimental testing of novel high-order composite pulses, which improve on existing protocols.

Chapter 6 introduces methods for characterising the stability of frequency standards, expressed in the vernacular of filter transfer functions. The traditional analytic approach to frequency standard variance calculations is extended to the case of locked local oscillators. The key tool for performing this extension, the novel ‘pair covariance transfer function’ that captures statistical correlations between two time-separated measurements, is derived.

Chapter 7 presents results on the stabilisation of frequency standards. The covariance transfer function derived in the previous chapter is used to develop a scheme for linearly combining multiple measurement outcomes in order to predict the trajectory of noise. This scheme produces improved feedback correction accuracy and hence improved LLO stability. Since this predictive scheme relies on spectral information about the noise, it is tested in a range of parameter regimes by numerical simulation. The success of the scheme in simulation motivates the development of the trapped-ion qubit system as an experimental emulator of frequency standards, which may be tuned within a wide range of control and noise parameter settings. The improved stability afforded by the predictive scheme is verified by experimental results.

Chapter 8 summarises the main contributions made to the field of precision quantum control in this thesis. On the basis of these contributions, it suggests fruitful directions for future research and applications of the results of the thesis.
Chapter 2

Experimental Platform: Ytterbium Ions in a Linear Paul Trap

Trapped ions are a proven architecture for extremely high-precision experiments in precision quantum control [7]. The primary advantages of trapped ions in this context are high-accuracy control over the electronic degrees of freedom, as well as the exceptionally long ion lifetimes and internal state coherence times [61]. Trapped ions have been a leading technology in time and frequency metrology from the 1990s to the present [19, 3, 52], and are an important platform for the development of quantum information processing [49, 60, 62] and quantum simulation [45, 10].

The trapped ions used in this thesis are $^{171}$Yb$^+$ ions in a linear Paul trap kept under ultrahigh vacuum (UHV) around $2 \times 10^{-10}$ Torr. A ‘cloud’ of ions is produced by the photoionisation of a beam of neutral Yb, and is Doppler-cooled in the centre of the trap by an ultraviolet laser at 369.5 nm. The multilevel electronic structure of Yb$^+$ is reduced in effect to a two-level system (the hyperfine ground state doublet) by using visible and infrared repump lasers. The cloud therefore forms an ensemble of identical two-level quantum systems (qubits). This hyperfine qubit with a transition at 12.6 GHz is coherently driven by unidirectional free space microwaves [71] and the occupancy of the excited $F = 1$ state is detected by a fluorescence shelving technique [17]. Fluorescence is measured with a photomultiplier tube and photon counter, and the hardware is centrally coordinated by a PC running WaveMetrics’ IGOR Pro.

This chapter is organised as follows. Section 2.1 outlines the design of the ion trap used in these experiments, including the basic derivation of the trapping pseudopotential. Section 2.2 describes the relevant electronic energy level structure of Yb$^+$, including the relationship between radiation polarisation and the spatial orientation of the ions’ magnetic dipole. Section 2.3 describes the optically-driven transitions used for ionisation, cooling, state preparation and detection, while section 2.4 describes the optical system that delivers the laser beams to the ion cloud. Section 2.5 describes the ion state measurement apparatus. Section 2.6 describes the setup used to deliver coherent microwaves for precision control of the qubit state. Section 2.7 presents a control-based normalisation technique for mitigating photon detection noise.

2.1 Trap design

The type of ion trap used for these experiments is a linear radiofrequency (RF) trap, also known as a Paul trap [79]. It was proven in the nineteenth century by Earnshaw [18] that a point charge cannot be confined by electrostatic forces alone, so the Paul trap uses a combination of static and oscillating electric fields to confine ions. The following summary of Fisk [19] explains how such an arrangement of fields produces confinement. Consider in one dimension an ion of mass $m$ and charge $q$, in the presence of a sinusoidally oscillating electric field with frequency $\Omega$ and position-dependent amplitude $E_0(y)$. The ion experiences a force
\[ F(t) = qE_0(y) \cos(\Omega t) \] \hspace{1cm} (2.1)

and so its position, given the initial condition \( y(0) = 0 \), is

\[ y(t) = -\frac{qE_0(y)}{m\Omega^2} \cos(\Omega t) \] \hspace{1cm} (2.2)

For sufficiently large \( \Omega \), the deviation \( |y - \bar{y}| \) of the ion from its average position is small, and the \textit{pseudopotential approximation} can be made. In this approximation, the electric force is written

\[
    F(t) = qE_0(\bar{y}) \cos(\Omega t) + q\frac{dE_0(\bar{y})}{dy} (y - \bar{y}) \cos(\Omega t)
\]

\hspace{1cm} (2.3)

\[
    = qE_0(\bar{y}) \cos(\Omega t) - \frac{q^2E_0(\bar{y})}{m\Omega^2} \frac{dE_0(\bar{y})}{dy} \cos^2(\Omega t)
\]

\hspace{1cm} (2.4)

where the second line is obtained by substituting in (2.2). Averaging (2.4) over a single cycle of the electric field oscillation gives

\[
    \bar{F}(\bar{y}) = -\frac{q^2E_0(\bar{y})}{2m\Omega^2} \frac{dE(\bar{y})}{dy}
\]

\hspace{1cm} (2.5)

Extending the problem to three spatial dimensions \( \vec{r} = (x, y, z) \) and defining the \textit{ponderomotive pseudopotential} \( F(\vec{r}) = q\nabla \Psi(\vec{r}) \) gives

\[
    \Psi(\vec{r}) = \frac{qE_0^2(\bar{r})}{4m\Omega^2}
\]

\hspace{1cm} (2.6)

Any electric field configuration that at some position satisfies \( \nabla \Psi = 0 \) and \( \nabla^2 \Psi > 0 \) can trap charged particles. Paul traps use a combination of static (DC) and oscillating (RF) potentials to satisfy these conditions, resulting in a quadrupole potential at the centre of the trap.

Prestage \textit{et al.} \cite{64} first demonstrated the use of a \textit{linear} Paul trap, consisting of four parallel rods acting as RF electrodes with the DC potentials applied by a pair of end caps. The advantage conferred by a linear geometry over the conventional hyperbolic geometry is that the pseudopotential minimum is extended along the trap axis, allowing more ions to be trapped. The resulting ion cloud has an ellipsoidal shape whose axial extent can be tuned from a few mm up to 1 cm by the DC potentials on the end caps, as opposed to the spherical cloud produced in a hyperbolic trap.

In the linear Paul trap used for these experiments, the trapping conditions are fulfilled with RF applied only to one diagonal pair of rods, shown schematically in Figure 2.1. For general operation, the RF frequency is set to 425 kHz and the RF amplitude to 150 V \textit{pp}. The other pair of rods have DC voltages applied to them for the purpose of \textit{shimming}, whereby spontaneous asymmetries in the trapping potential are compensated for by applying a DC bias perpendicular to the RF electric field. Such asymmetries are usually produced by the accumulation of unwanted charge on conducting surfaces inside the vacuum chamber or trap mounting. Shimming is done by regularly optimising the DC rod voltages in order to centre the ion cloud in the trap, and can be enhanced by applying a DC bias to the RF potential.

\subsection{2.2 Yb$^+$ ion energy level structure}

The ytterbium ion is an attractive choice for quantum control and frequency standard experiments because the relevant optical transitions can be accessed with commercial lasers, allowing for fast and efficient cooling of the ion cloud and preparation and detection of its electronic state \cite{61}. The
Figure 2.1: A schematic diagram of the linear Paul ion trap setup used in these experiments. The end caps have holes in the centre to allow laser beams to be incident on the cloud in the axial (Y) direction. The free-space microwaves from the horn and lens combination propagate radially (X), while the aligning magnetic field is oriented 45° in the XZ plane.

A hyperfine qubit is defined to be the $F = 0 \rightarrow 1, m_F = 0 \rightarrow 0$ transition of the ground state $^2S_{1/2}$, which is known as a ‘clock transition’ because it is first-order insensitive to magnetic fields, making it useful for frequency standard applications [21, 61]. Borrowing notation from quantum information, the qubit states are defined $|0\rangle \equiv |^2S_{1/2}(F = 0, m_F = 0)\rangle$ and $|1\rangle \equiv |^2S_{1/2}(F = 1, m_F = 0)\rangle$.

Figure 2.2 shows the energy level structure of the Yb$^+$ ion. The $^2S_{1/2}$ and $^2P_{1/2}$ states do not form a closed subsystem of the Yb$^+$ electronic manifold, as the $^2P_{1/2}(F = 1)$ state decays to the $^2D_{3/2}(F = 1, 2)$ states with 0.5% probability. Decay out of the $^2P_{1/2}$ manifold causes full population of the undesired $^2D_{3/2}$ state in less than a second, given the ion cloud sizes used in this experiment. Furthermore, collision of the ions with background gas drives the $^2D_{3/2} \rightarrow ^2D_{5/2}$ transition, from which the ions decay to the extremely long-lived $^2F_{7/2}$ state [55, 61]. In order to recover these ions into the desired manifold, repump lasers are used, as described in Section 2.3.3.

The detailed $S-P$ level diagram in Figure 2.4 shows the hyperfine splitting of $^2S_{1/2}$ and $^2P_{1/2}$ at 12.643 GHz and 2.105 GHz respectively, with each $F = 1$ level further Zeeman split into a $m_F = -1, 0, 1$ triplet. As seen in the next section, the $S - P$ transition is required for both state detection and cooling of the ion cloud.

The qubit is defined by the magnetic dipole transition $|0\rangle \rightarrow |1\rangle (F = 0 \rightarrow 1)$ that exists in the ground state manifold. In order to drive the qubit transition uniformly over the whole cloud, the magnetic dipole must be spatially oriented. This requires the application of a static, uniform magnetic field across the cloud. This field is achieved by three pairs of Helmholtz coils experiencing fixed DC to produce a homogeneous field across the ions of strength 1.8 Gauss, as depicted in Figure 2.3. The application of this field produces a small Zeeman triplet splitting of the $|1\rangle$ state by some tens of MHz. The entire trap and vacuum chamber is magnetically insulated from ambient magnetic fields by a Ni-Co shield. The induced spatial alignment allows linearly polarised optical and microwave radiation to preferentially target all three Zeeman-split states of $|1\rangle$ (optical cooling beam), or only the $|1\rangle (m_F = 0)$ (microwave driving beam), as outlined in section below.
Figure 2.2: Energy level structure, showing transitions in the UV (purple arrows), visible (red arrows) and IR (green arrows) regions of the spectrum. Thin grey lines indicate spontaneous decay paths between levels. The dashed black lines show transitions due to collisions with background gas that provide a path to the undesired $^2F_{7/2}$ states. The term symbols of the $^3[3/2]_{1/2}$ and $^1[5/2]_{5/2}$ states indicate that two electrons are excited and couple to each other as well as to the atomic core, a departure from the usual LS-coupling [61].

2.3 Driving of ion optical transitions

2.3.1 Two-stage photoionisation

To trap an ion cloud, a filament of isotopically-enriched Yb is heated, producing a neutral beam of predominantly $^{171}$Yb through the centre of the trap. During this loading stage, two overlapping UV beams at 398.9 nm and 369.5 nm cross the Yb beam and via a two-stage photoionisation process produce Yb$^+$. The 398.9 nm photon excites a bound electron from the ground state to the $^1P_1$ excited state and the 369.5 nm photon excites the electron into the continuum of unbound states [61]. The number of ions in a trapped cloud depends on the density of the neutral Yb beam, which is tuned via the current applied to the filament. In this manner, large ion numbers between $10^3$ and $10^4$ can be obtained, which results in an excellent measured signal to projection noise ratio [36].

2.3.2 Doppler cooling of ion cloud

Doppler cooling of the ion cloud is achieved by a beam of 369.5 nm light with approximately 100 $\mu$W of optical power which is red-detuned from the $^2S_{1/2}(F = 1) \rightarrow ^2P_{1/2}(F = 0)$ optical transition by 10 MHz, half its natural linewidth. The ions experience stimulated photon absorption preferentially, since they are more likely to absorb a photon if the ions and photons are moving in opposite directions. Since the ions re-emit isotropically, the momentum component in the opposing direction is reduced, and after many absorption and emission events, the overall ion kinetic energy is absorbed by the restoring force of the trap. This process cools the ions down to a ‘Doppler limit’ set by the photon recoil energy [82]. In the experiment, the cooling is achieved by scanning the 369.5 nm laser frequency across 200 MHz on the red side of the optical transition in a sawtooth pattern with a cycle time of 10 s. The UV cooling beam is equally split into a ‘straight’ and ‘oblique’ beam before
entering the trap and recombining at an angle in the trap centre, in order to increase Doppler cooling efficiency by targeting a larger section of the ions’ velocity space. It is sufficient for these experiments to work near the Doppler cooling limit, and so additional cooling techniques such as resolved sideband cooling are not necessary [37].

Since there is a non-negligible probability of off-resonant driving and decay to $^2S_{1/2}(F = 0)$ and $^2P_{1/2}(F = 1)$ levels, sidebands are added to the cooling beam at 14.75 GHz using the second-order modulation of a 7.374 GHz electro-optical modulator (a New Focus free-space EOM, model number 4851-02). The combination of 369.5 nm carrier and the 14.75 GHz sideband allows Doppler cooling of all states in the $S$ and $P$ manifolds except for the $^2S_{1/2}(F = 1, m_F = \pm 1)$ Zeeman split states. To couple these Zeeman split states to the $F = 0$ states and hence allow them to be cooled, it is necessary to tailor the polarisation of the cooling beam. In order to drive both the $\Delta m_F = 0$ transition, which requires linearly polarised photons, and the $\Delta m_F = \pm 1$ transitions, which requires left and right circularly polarised photons, the cooling beam’s polarisation must be chosen with respect to the alignment of the qubit dipole axis. The cooling beam is linearly polarised at 45° to the dipole axis, so that it is decomposed into parallel and perpendicular components with respect to that axis. The parallel component drives the $\Delta m_F = 0$ transition while the perpendicular component is further decomposed into left and right circular components, which drive the $\Delta m_F = \pm 1$ transitions [55]. Thus the $m_F = \pm 1$ states are coupled to relevant $m_F = 0$ states and can be Doppler cooled. An
Figure 2.4: \( S \rightarrow P \) transitions in Yb\(^+\). Thick solid lines indicate resonant transitions driven by the carrier frequencies while thin solid lines indicate transitions driven by sideband frequencies. Doppler cooling; purple arrows show the 369.5 nm stimulated transitions: the three \( \Delta m_F = -1, 0, 1 \) transitions at resonance and the one \( \Delta m_F = 0 \) on the 14.75 GHz sideband. Light grey arrows show spontaneous decay paths; all \( P \rightarrow S \) transitions are permitted by selection rules except the \( (F = 0) \rightarrow (F = 0) \) and \( (F = 0, m_F = 0) \rightarrow (F = 1, m_F = \pm 1) \) decay transitions. The use of the 14.75 GHz sideband and polarisation alignment allows Doppler cooling of all the hyperfine and Zeeman states in the \( ^2S_{1/2} \) and \( ^2P_{1/2} \) manifolds. State initialisation; 369.5 nm beam is modulated by 2.105 GHz sidebands, which excite the \( (F = 1) \rightarrow (F = 1) \) transitions. The \( ^2S_{1/2}(F = 1) \rightarrow ^2P_{1/2}(F = 0) \) resonant transitions and \( ^2P_{1/2}(F = 0) \rightarrow ^2S_{1/2}(F = 1) \) spontaneous decay are present without contributing to the initialisation cycle, and so for clarity they are not shown in this middle sub-figure. After excitation to \( ^2P_{1/2}(F = 0) \) by the sideband transition, the qubit decays into the |0\> hyperfine ground state without being excited further, producing state initialisation in |0\>. State detection; no sidebands are applied to the 369.5 nm, resulting in driving only of the \( ^2S_{1/2}(F = 1) \rightarrow ^2P_{1/2}(F = 0) \) transition. This forms a closed subspace that prevents change in the relative population of |0\> and |1\>, resulting in an unambiguous qubit state measurement. Transitions are not shown to scale.

energy level diagram depicting the cooling transitions appears in Figure 2.4.

2.3.3 Depopulation of undesired states

To maintain the ion state in the desired subspace, two ‘repump’ lasers are applied. An IR laser at 935.2 nm with approximately 4 mW of optical power drives the \( ^2D_{3/2}(F = 2) \rightarrow ^2[3/2]_7/2(F = 1) \) transition, with an EOM-generated (a fibre EOM from EOspace) sideband at 3.067 GHz driving the \( ^2D_{3/2}(F = 1) \rightarrow ^3[3/2]_7/2(F = 0) \) transition. From the \( ^2[3/2]_7/2 \) state the ions rapidly decay to the ground state \( ^2S_{1/2} \) and are returned to the cooling cycle. To depopulate \( ^2F_{7/2} \) state, a visible red laser alternating between 638.610 nm and 638.616 nm is overlapped with the repump IR beam. The rate of decay into the \( ^2F_{7/2} \) state is sufficiently slow that the hyperfine-split levels can be depopulated by alternating between the two transition frequencies every 30 s. The red beam drives the \( ^2F_{7/2} \rightarrow ^1[5/2]_5/2 \) transition (details of the hyperfine splittings are shown in the figure), from which there is rapid decay back into the \( ^2D_{3/2} \) states.
2.3.4 State initialisation and detection

The ion state is initialised by inducing decay to the $^{2S_{1/2}}(F = 0)$ state (i.e. $|0\rangle$), which is achieved by introducing 2.105 GHz EOM-generated sidebands (a free-space EOM from New Focus, custom AR-coated model number 4431-01) onto the cooling beam and applying the two repump beams. The 7.374 GHz sidebands are absent from the cooling beam during initialisation, so that there is no driven coupling from $|0\rangle$ to any other state. This configuration results in initialisation of all the ions to $|0\rangle$. Detection of the qubit state is achieved by coupling the $|1\rangle$ state to $^{2P_{1/2}}(F = 0)$ using 369.5 nm light with no sidebands. This transition is closed, resulting in a large number of photons scattered from a repeated absorption and emission process and hence an improvement in the fluorescence signal in contrast to driving to $^{2P_{1/2}}(F = 1)$ [20]. An energy level diagram depicting the state initialisation and detections transitions appears in Figure 2.4.

Since the frequencies of these sidebands must be very precisely determined, RF signals in the GHz regime are synthesised from a 10 MHz RF reference using a pair of Hittite micro synthesisers (model HMC-C070 for the 7.374 GHz signal and HMC-C083 for the 2.105 GHz signal) and a Mini-Circuits voltage-controlled oscillator (VCO, for the 3.067 GHz signal). The frequencies of these synthesisers are set via a USB interface from National Instruments, and monitored on a Hewlett-Packard frequency counter.

2.4 Laser system

In order to achieve the efficient and accurate driving of the optical transitions covered in the previous section, the optical system must fulfil the following criteria:

- narrow linewidth < 5 MHz
- long-term frequency stability
- precisely tunable sidebands

The sources for all four laser frequencies are external cavity diode lasers (ECDL) from MOGLabs, which are frequency-locked using a commercial wavemeter from High-Finesse/Ångstrom running in multi-channel mode. The sidebands are added to the relevant beams by electro-optical modulators (EOM) driven by synthesised RF power at the required GHz frequencies. The application and removal of sidebands and beamlines on the sub-millisecond time scales of the experiments are performed by TTL-triggered switching of the optical modulators. A more detailed description of each part of the optical system follows.

2.4.1 External cavity diode lasers

All the frequencies used in this optical system: UV at 369.5 nm and 398.9 nm, IR at 935.2 nm and visible at 638.6 nm, are produced by semiconductor diode lasers coupled to external cavities in a Littrow configuration [38]. The ECDLs are from MOGLabs with model number ECD-003, with controller boxes from MOGLabs with model number DCL-202. For the generation of 369.5 nm, the ECDLs are a low-cost, low-power alternative to previous techniques involving a high-power Ti:sapphire laser and lossy frequency doubling techniques [22]. The diode consists of a semiconductor heterostructure which acts both as a light-emitting part and a gain medium. Emitted photons pass through a collimator and are incident on a diffraction grating whose angle is piezoelectrically controlled; this forms the external cavity.

The arrangement of internal and external cavities produces three overlapping mode structures: the grating modes, the internal cavity modes and the external cavity modes. The output frequency of the ECDL is determined by the combined mode with the highest power. Since the three mode structures are shifted by separate physical mechanisms (grating modes by the piezo voltage, internal modes by
the current through the diode, external modes by an overall temperature control of the cavity), the experimentalist is able to select the desired mode and tune it in a range of $\sim 5$ GHz. [38]

### 2.4.2 Laser frequency stabilisation

The frequencies of the four lasers are cyclically measured using a wavelength meter, commonly referred to as a wavemeter, from High-Finesse/Ångstrom with model number WSU U-10, which can operate in an multi-channel switching mode to monitor up to eight frequencies in tandem. The wavemeter is a relative frequency reference that is calibrated to an absolute Helium-Neon (HeNe) laser reference, achieving 1 MHz relative and 10 MHz absolute frequency accuracy [38]. The wavemeter itself has only a front and back fibre optical port, so two external four-channel switches are triggered by the wavemeter to multiplex the four input beams into the wavemeter. The IR and visible beams are sent through a commercial fibre optical switch that TTL-triggered by the wavemeter. The two UV beams are switched using a custom-built free-space switch: a pair of AOMs pass the two beams on an eight-channel cycle coordinated by a flip-flop-based circuit and TTL-triggered by the wavemeter, as shown in Figure 2.6.

By measuring the laser frequencies in real time, the wavemeter can be used to lock them to the desired set points. The frequency measurements are delivered to a PC, which acts as a software PID controller that sends a command back to the wavemeter to output a control voltage. The control voltages are routed to each laser’s piezoelectric control, closing the feedback loop and allowing stabilisation of the laser’s output frequency. In switching mode the wavemeter applies corrections to each laser frequency approximately once a second, which results in deviation at the sub-MHz level that is acceptable for these experiments, without the need for more sophisticated stabilisation at higher bandwidths such as Pound-Drever-Hall locking or polarisation spectroscopy [38, 50]. This is possible because intrinsic current noise in the controller is so low that additional linewidth narrowing
Figure 2.6: Switch and wavemeter setup. In eight-channel switch mode, the wavemeter accepts light from either the front or back port, sending the measurement outcome for each channel to the PC via USB (solid black arrow) and trigger the switch and flip-flop circuit by TTL pulses (dotted arrows). The fibre-optic switch operates on a four-stage cycle, sending in IR, red and no light in series; the fibre components are shown as brown solid lines. The flip-flop circuit operates on an eight-stage cycle, sending TTL pulses to two RF switches at the second and third out of eight triggers. The RF switches regulate the 70 MHz driving of two free-space AOMs, which act as ‘shutters’, rapidly producing and removing first-order diffraction beams that continue on to a combiner and are overlapped into a fibre-coupler. The effect of this switch-AOM setup is allow the two UV beams to enter the front wavemeter port in series, as triggered by the flip-flop circuit. Since light entering the front port overrides measurements taken at the back port, the net effect of this two-port setup is that each of the four beams (369.5 nm, 398.9 nm, 935.2 nm and 638.6 nm) are measured on their own channels. On the basis of the measurements, the PC calculates a PID control value which is sent back to the wavemeter, in order to piezo-control each laser.
via current feedback and an external Fabry-Perot optical cavity is unnecessary [50]. These experiments represent the first Doppler-limited cooling using the output of a bare ECDL without additional linewidth narrowing.

2.5 Measurement system

When sufficiently cooled, the ion cloud fluoresces at 369.5 nm. During the loading and initial cooling stages, a CCD video camera (Andor Solis) with a 369.5 nm UV filter is used to precisely determine the \( ^2S_{1/2} \rightarrow ^2P_{1/2} \) resonance frequency and to estimate the size of the cloud. The fluorescence intensity of the cloud is directly proportional to the probability of observing the qubit in the \( |1\rangle \) state, so the measured intensity of scattered photons is used as a proxy for a projective \( Z \)-basis measurement of the qubit state. A photomultiplier tube (PMT) from Products for Research and a gated photon counter (from Stanford Research Systems with model number SR400) linked to the experiment PC via an RS-232 serial connection, is used to measure ion fluorescence. The photons are counted for a fixed gate period, generally 1 ms, giving a more accurate measurement of fluorescence intensity than possible with the CCD camera. The accuracy of the counter photon number is enhanced by a Semrock filter FF01-370/6 placed on the aperture of the PMT that transmits light at 369.5 nm, within a bandwidth of 10 nm, reducing the effect of background photon noise. In order to switch between CCD camera and photon counter imaging of the cloud, the two devices are placed on a pair of precision translation stages (from ThorLabs with model number NRT100E). By alternating the translation stages between two sets of optimised settings, the user can choose to align either the CCD camera or the photon counter with the static ion trap. The image is focussed using a 100mm diameter Knight optical lens with 160mm focal length (model number LPV160100) followed by an 80mm diameter lens with 100mm focal length.

2.6 Coherent control of the qubit

A useful method of visualising the qubit state is the image of the Bloch sphere, where a pure state

\[
|\psi\rangle = \cos (\theta/2) |0\rangle + \sin (\theta/2) e^{i\phi} |1\rangle
\]

(2.7)

is represented as a vector from the centre of the sphere to its surface, where \( \theta \) and \( \phi \) are the polar and azimuthal angles on the sphere. This geometrical interpretation is possible due to the homomorphism between the SU(2) group symmetry of the qubit state space and the SO(3) symmetry of the 3D geometrical space [24].

Coherent driving of the qubit state, say from \( |0\rangle \) to \( |1\rangle \), may be represented as rotations on the Bloch sphere. For example, phase-coherent driving of the qubit by the microwave oscillator results in rotation of the Bloch vector about some axis in the \( XY \) plane, while dephasing perturbations of the qubit state result in random rotations about the \( Z \) axis. A visualisation of such a driven rotation on the Bloch sphere is shown in Figure 2.7. The following section derives the relationship between constant uniform driving of the qubit state and the resulting rotation of the qubit state, which is known as ‘Rabi oscillation’. The term ‘\( \pi \) time’ refers to the time taken to drive a \( \pi \)-rotation on the Bloch sphere, and as such is an inverse measure of Rabi rate.

2.6.1 Derivation of qubit Rabi oscillation

Since the quantum system targeted by these experiments is the hyperfine qubit that resides in the ground state \( ^2S_{1/2} \) manifold, the problem of microwave field-ion state interaction can be formulated as the ‘two-level Rabi problem’. The solution is found by a time-dependent perturbation theory approach to the response of a quantum dipole system to a coherent classical field. The field-qubit interaction produces a coherent oscillation of the qubit state on a time scale set by the amplitude of
Figure 2.7: Driven rotation on the Bloch sphere. The phase of the driving oscillator determines the axis of rotation $\hat{n}$, while the amplitude of the driving field determines the rate of rotation (the ‘Rabi rate’). For a given driving time, the rate determines the arc length of the Bloch vector’s trajectory $\theta(t)$. This figure is based on that found in [24].

the field, known as ‘Rabi oscillation’ or ‘Rabi flopping’.

The following derivation is based on the summary in [71]. Starting from a discrete multi-level quantum system, an arbitrary state $|\Psi\rangle$ may be written as a linear combination of energy eigenstates $|n\rangle$, defined as

$$\hat{H}_q |n\rangle = E_n |n\rangle$$  \hspace{1cm} (2.8)$$

where $\hat{H}_q$ is the quantum system’s time independent Hamiltonian. The effect of interaction with a time-varying field is most simply written by expressing the total Hamiltonian as the sum

$$\hat{H}(t) = \hat{H}_q + \hat{H}_i(t)$$  \hspace{1cm} (2.9)$$

where $\hat{H}(t)$ is the total Hamiltonian and $\hat{H}_i(t)$ is the time-dependent interaction Hamiltonian. The perturbative approximation lies in assuming that the interaction is sufficiently small that the state can be expressed as a normalised superposition of the eigenstates of $\hat{H}_q$

$$|\Psi(t)\rangle = \sum_n c_n(t)e^{-iE_n t/\hbar} |n\rangle$$  \hspace{1cm} (2.10)$$

where the coefficients $c_n(t)$ are in general complex. Substituting this ansatz into the time-dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle$$  \hspace{1cm} (2.11)$$

and left-multiplying by the eigenstate $\langle m|$ gives, after some manipulation

$$i\hbar \dot{c}_m(t)e^{-iE_m t/\hbar} = \sum_n c_n(t)e^{-iE_n t/\hbar} \langle m| \hat{H}_i |n\rangle$$  \hspace{1cm} (2.12)$$
The matrix element $H_{mn}$ of the interaction Hamiltonian is defined: $H_{mn} = \langle m | \hat{H}_i | n \rangle$, and the further restriction is applied that since $\hat{H}_i$ captures interaction with a classical field, the matrix $H_{mn}$ is Hermitian so that $H_{mn} = H_{nm}^*$. Reducing the dimension of $H_{mn}$ to the two-level system (a qubit) relevant to this physical system produces a pair of coupled ordinary differential equations (ODE) describing the time evolution of the qubit state

\begin{align*}
\dot{c}_1(t) &= c_0(t) H_{10} e^{i \omega_{10} t} \\
\dot{c}_0(t) &= c_1(t) H_{10}^* e^{-i \omega_{10} t}
\end{align*}

where $\omega_{10} = (E_1 - E_0)/\hbar$ and $|0\rangle$ and $|1\rangle$ label the ground and excited energy states.

Assuming a coherent dipole interaction with a magnetic field linearly polarised and aligned with the quantisation axis of the qubit, the interaction Hamiltonian can be written

\begin{equation}
\hat{H}_i = -\vec{\mu} B \cos (\omega t + \phi)
\end{equation}

where $\vec{\mu}$ is the qubit magnetic dipole moment and $B$ and $\phi$ are the amplitude and phase of the driving magnetic field. Making the magnetic dipole approximation, which consists of assuming that variations in the magnetic field strength are insignificant on the scale of the qubit’s spatial wavefunction, is justified in this experimental system [71]. Substituting this dipole interaction Hamiltonian into the coupled ODEs gives

\begin{align*}
\dot{c}_1(t) &= c_0(t) \frac{i \Omega}{2} \left( e^{i(\omega+\omega_{10})t} e^{i\phi} + e^{-i(\omega-\omega_{10})t} e^{-i\phi} \right) \\
\dot{c}_0(t) &= c_1(t) \frac{i \Omega^*}{2} \left( e^{i(\omega-\omega_{10})t} e^{i\phi} + e^{-i(\omega+\omega_{10})t} e^{-i\phi} \right)
\end{align*}

where the complex resonant Rabi rate is defined $\Omega \equiv \langle 1 | \vec{\mu} | 0 \rangle B/\hbar$. To solve this coupled ODE system, a further approximation is required. The rotating wave approximation assumes that the frequency detuning $\Delta \equiv \omega - \omega_{10}$ is negligible compared to the nominal frequency $\Delta \ll \omega$ so that the frequency sum components $\omega + \omega_{10}$ can be considered to average to zero on the time scale of the frequency detuning components $\Delta$. Given the rotating wave approximation, the coupled ODEs can be rewritten

\begin{align*}
\dot{c}_1(t) &= c_0(t) \frac{i \Omega}{2} e^{-i \Delta t} e^{-i\phi} \\
\dot{c}_0(t) &= c_1(t) \frac{i \Omega^*}{2} e^{i \Delta t} e^{i\phi}
\end{align*}

These ODEs can be combined into a single second-order ODE in $c_1(t)$

\begin{equation}
\ddot{c}_1(t) + i \Delta \dot{c}_1(t) + \left| \frac{\Omega}{2} \right|^2 c_1(t) = 0
\end{equation}

whose general solution is

\begin{equation}
c_1(t) = e^{-i \Delta t} \left( a e^{-i \Omega t/2} + b e^{i \Omega t/2} \right)
\end{equation}
where $a$ and $b$ are coefficients that depend on the initial state $c_1(0)$ and $\Omega_R = \sqrt{|\Omega|^2 + \Delta^2}$ is called the ‘generalised’ Rabi rate, which for zero detuning reduces to the resonant Rabi rate $|\Omega|$.

Since a solution is required for an arbitrary initial state, the time evolution of $c_0(t)$ and $c_1(t)$ is written as a linear transformation by a ‘rotation matrix’ $R(t)$

$$
\begin{bmatrix}
c_1(t) \\
c_0(t)
\end{bmatrix} =
\begin{bmatrix}
R_{11}(t) & R_{10}(t) \\
R_{01}(t) & R_{00}(t)
\end{bmatrix}
\begin{bmatrix}
c_1(0) \\
c_0(0)
\end{bmatrix}
$$

This matrix equation can be solved for an arbitrary initial state by applying the general solution (2.21) and setting the initial state to be two basis states $[1 0]$ and $[0 1]$. The rotation matrix is therefore

$$
R(t) = \begin{bmatrix}
e^{-i\Delta t/2}(\cos (\Omega_R t/2) + \frac{i\Delta}{\Omega_R} \sin (\Omega_R t/2)) & \frac{i\Omega^*}{\Omega_R} e^{i\Delta t/2} e^{i\phi} \sin (\Omega_R t/2) \\
e^{i\Delta t/2}(\cos (\Omega_R t/2) - \frac{i\Delta}{\Omega_R} \sin (\Omega_R t/2)) & e^{i\Delta t/2}(\cos (\Omega_R t/2) - \frac{i\Delta}{\Omega_R} \sin (\Omega_R t/2))
\end{bmatrix}
$$

which in the case of a resonant driving field $\Delta = 0$ reduces to

$$
R(t) = \begin{bmatrix}
\cos (\Omega_R t/2) & i e^{i\phi} \sin (\Omega_R t/2) \\
i e^{-i\phi} \sin (\Omega_R t/2) & \cos (\Omega_R t/2)
\end{bmatrix}
$$

with $\Omega_R = |\Omega|$. This form of the rotation matrix completely captures the effect of coherently driving a qubit. From the definition of the Rabi rate it can be seen that the rate of driven transition between the two states is proportional to the amplitude $B$ of the driving field, while ‘axis of rotation’ in the Bloch sphere picture is given by the phase of the driving field $\phi$.

### 2.6.2 Microwave setup for driven qubit control

The qubit state transition $|0\rangle \leftrightarrow |1\rangle$ is coherently driven by microwaves at 12.6 GHz, whose linear polarisation is parallel aligned to the qubit dipole axis. In order to accurately and precisely control the ion state, there are several criteria that the microwaves must fulfil:

- high power for rapid driven Rabi rate on the order of $\Omega \sim 100$ kHz
- spatial homogeneity over the ion cloud to maintain the coherence of the ensemble
- precise and arbitrary modulation of phase and amplitude
- excellent frequency, power and polarisation stability

The microwaves are generated by an Agilent vector signal generator (VSG) with model number E8267D and the UNY option for enhanced ultra-low phase noise, amplified by an 18 dB RF amplifier (from Microsemi with model number AML618P1802) and delivered as directed free-space waves via a conical microwave horn and dielectric lens (from Flann Microwave with model number CL320-4901) [71]. The overall microwave setup is schematically depicted in Figure 2.8. A primary benefit of using the VSG is that the continuous-wave output may be arbitrarily phase and amplitude modulated, either by a software link or by an external arbitrary waveform generator (AWG). The experiment PC uses a 16-bit Pulseblaster (from Spincore with model number DDS-IV 1000) to produce 5 V TTL pulses that trigger the VSG, producing sharply rectangular gated pulses, and in the case of FM, trigger the AWG to start applying the modulating waveform. The Pulseblaster can be preprogrammed by the PC to execute a complex series of triggers that manage the whole apparatus including microwave and optical components, and these triggers are synchronised to the 10 MHz Cs reference, which is supplied by the National Measurement Institute and cleaned using a Wenzel crystal.

The VSG produces a carrier RF signal with mHz precision and is also frequency-stabilised to the 10 MHz Cs reference. The phase noise specification of the VSG output, which can be quantified in
terms of power at a fixed offset from the carrier, is given by Agilent as -138 dBc/Hz at 10 kHz and -141 dBc/Hz at 100 kHz offset. After amplification, the maximum achievable microwave power is 33 dBm which corresponds to a measured minimum $\pi$ time $\tau_\pi = 4 \mu s$, though most experiments are operated at $\tau_\pi > 25 \mu s$. The use of an external gate trigger supplied by a TTL signal from the Pulseblaster, which achieved via the pulse modulation setting on the VSG, allows these rapid $\mu s$ pulses to be precisely timed. The TTL pulse jitter and shape can be examined using high-bandwidth oscilloscope and the fidelity of the output microwave pulses can be checked using an Agilent MXA Vector Analyser N9020A.

Several methods could have been used to deliver microwaves to trapped ions, including applying microwaves to the trap rods themselves, open-ended waveguides or microwave horn antennae [71]. The benefit of the horn and lens combination used in this setup is that it produces a highly directed beam, which maximises the power directly incident on the ions and minimises undesired reflections from the vacuum chamber walls. Thus the criteria of high power and spatial homogeneity are well met by the horn and lens. The microwave horn acts as a waveguide whose diverging geometry reduces the reflection at the free-space interface, while the dielectric lens focuses the microwaves into a narrow waist near the trapped ions.
2.7 Improved photon detection accuracy by Bayesian normalisation

Fluctuations in the 369.5 nm laser amplitude and detector shot noise lead to errors in the qubit state measurement. To mitigate the effect of amplitude fluctuations slower than the measurement time, a normalisation procedure is employed. Before the measurement of the desired state $|\psi\rangle$, the $|1\rangle$ ‘bright’ and $|0\rangle$ ‘dark’ states are prepared and measured. A linear interpolation is performed between the bright state count $B$ and dark state count $D$ in order to cancel the effect of slow laser amplitude drifts on the measured fluorescence of $|\psi\rangle$.

To mitigate the high-frequency shot noise, an iterative Bayesian estimation scheme is employed. Identical sets of normalisation and state measurements are performed up to a desired number of iterations $I$. A modified form of Bayes’ rule is used:

$$ P(\theta|c_i) = \frac{P(c|\theta)P(\theta|c_{i-1})}{\int_0^{\pi} P(c|\theta)P(\theta|c_{i-1})d\theta} \quad (2.25) $$

where $c_i$ is the measured photon count on the $i$th iteration and $\theta$ is the Bloch vector inclination from $|0\rangle$ to $|1\rangle$. The prior state probability density $P(\theta)$, initially assumed to be uniform, is iteratively refined $I$ times by applying the rule. The likelihood function $P(c|\theta)$, which captures the detector noise probability, is experimentally verified to be Gaussian-distributed within the bounds of the bright and dark state normalisation counts [70]:

$$ P(c|\theta) = \exp\left[ -\left( \frac{\bar{D} + \frac{\bar{B}-\bar{D}}{\frac{\pi}{\sigma_D}}\theta}{\sigma_B + \frac{\sigma_B-\sigma_D}{\pi}\theta} \right)^2 \right] \quad (2.26) $$

where $\bar{B}, \bar{D}$ are the mean bright and dark state counts, while $\sigma_B, \sigma_D$ are the standard deviations over the set of iterations. The final estimate for $\theta$ is found by taking the expected value of the posterior after all the iterations are complete, which gives the result of the projective measurement with greater than 98% accuracy [70].
Chapter 3

Semiclassical stochastic noise in quantum systems

In order to achieve precision control of the systems of interest, it is necessary to achieve a detailed characterisation of the dominant sources of noise. The quantum control community has a particular interest in stochastic, non-Markovian, universal qubit noise models [70], which are semiclassical models that capture many features of real noise environments [24]. The resulting qubit dynamics are non-dissipative, non-entangling and non-depolarising, which means that they can be modelled as unitary evolution of a single qubit. It is desirable to quantify this noisy evolution by quantities accessible in experiment. A convenient measure to use in this regard is the power spectral density (PSD), which is a frequency-domain function that captures the autocorrelation in the noise (also referred to as its ‘colour’). The PSD of a noisy signal can be easily inferred from spectral diagrams measured on a signal analyser.

A key task in quantum control is to produce techniques for error-robust control, taking into account information such as the PSD. The action of arbitrary control operations on the qubit may be represented in the frequency domain by filter transfer functions, well known in classical control theory and frequency metrology [14, 5, 66]. An important advantage of working with filter transfer functions is ease of use: the time-domain convolution of noise trajectories and response functions is transformed via the Wiener-Khinchin theorem, proven in this chapter, into a product of frequency domain quantities that may be straightforwardly evaluated. In this framework, the accumulation of error during a control protocol in a known noise environment is captured by metrics that are defined as the overlap integral of the transfer function of the control and the PSD of the noise. This transfer function framework allows for convenient calculation of error due to noise and for straightforward analysis of the error-suppressing properties of different control protocols.

The purpose of this chapter is to provide the relevant mathematical background to the control protocols used in later chapters. The chapter is organised as follows. Section 3.1 outlines the statistical basis for the frequency-domain approach of this thesis, rigorously defining concepts of ensemble, autocorrelation and ergodicity. Section 3.2 gives a first-principles derivation of the PSD that is a key quantity that captures the spectral features and correlations in the noise processes considered here. Section 3.3 gives a proof of the Wiener-Khinchin theorem that states that the PSD and the time-domain autocorrelation function form a Fourier pair.

3.1 Spectral character of noise statistics

In the quantum systems of interest, it is the statistical properties of an ensemble that are the most relevant and easily accessible [19, 6]. A fundamental reason for this is that projective measurement of a quantum system causes the wavefunction to collapse randomly into one of its eigenstates [73], so to achieve a reliable estimate of the state it is necessary to take an ensemble of measurements. Furthermore, since the relevant noise processes are stochastic, any robust characterisation of them
must be found by extracting features that are invariant over an ensemble of realisations, effectively ‘averaging over’ the stochasticity. Such statistical measures are of central importance to precision metrology and quantum measurement [66, 83]. The following derivation elaborates on the treatment of the PSD given in [56].

The main control problems of interest to this thesis involve stochastic noise processes that degrade the accuracy of driven manipulation of the qubit state. A generic time-domain continuous noise variable \( y(t) \) is used in the following derivation; its specific definition depends on the type of experiment. Since \( y(t) \) is a random function of time, it is different for every realisation of an experiment. Such a realisation is referred to in this thesis as a \textit{run} and a set of runs is referred to as an \textit{ensemble}; generally the former is indexed by \( r \) and the latter denoted by \( \mathcal{E} \), where the ensemble’s cardinality (number of runs) is written \(|\mathcal{E}|\). Often the ensemble has infinite cardinality and the characteristics of \( y(t) \) averaged for this infinite \( \mathcal{E} \) are assumed to reproduce the statistics of a single run of \( y(t) \), consistent with the frequentist interpretation of probability [29]. The aim is to describe the spectral character of the statistics of \( y(t) \), since such a description is more robust and informative than time-domain measurements of particular realisations.

The notation used for a mean of a stochastic function \( f(a) \) over an infinite ensemble is \( \mathbb{E}[F] \) where \( F \) is a random variable whose realisations are the values of \( f(a) \) for each run \( r \). The mean of a particular run of that function \( f_r(a) \) over its domain is written \( \langle f_r \rangle_a \). The definitions of these two types of mean are

\[
\mathbb{E}[F] \equiv \int_{\Omega} F p(dF) \tag{3.1}
\]

\[
\langle f_r \rangle_a \equiv \lim_{b \to \infty} \frac{1}{b} \int_0^b f_r(a) da \tag{3.2}
\]

where \( \Omega \) is the sample space of \( F \), \( p(dF) \) is the probability of obtaining the outcome in the range \([F, F + dF]\) (since it is assumed that the range of \( f(a) \) is a subset of \( \mathbb{R} \), \( f(a) \) has domain \( a \in [0, \infty) \)) and \( f_r(a) \) refers to the realisation of \( f(a) \) on the \( r \)th run. The subscript indexing the run is often omitted in general statements about the characteristics of \( f(a) \) not peculiar to individual runs. \( \mathbb{E}[F] \) is generally written \( \mathbb{E}[f(a)] \) for convenience.

Both \( \mathbb{E}[f(a)] \) and \( \langle f_r \rangle_a \) are ideal quantities that cannot be measured directly. Therefore it is assumed that they can be accurately estimated by \( \mathbb{E}[\hat{f}(a)] \) and \( \hat{f}_r \) where

\[
\mathbb{E}[\hat{f}(a)] \equiv \frac{1}{|\mathcal{E}|} \sum_{r \in \mathcal{E}} f_r(a) \tag{3.3}
\]

\[
\hat{f}_r \equiv \frac{1}{b} \int_0^b f_r(a) da \tag{3.4}
\]

such that the estimators converge to the ideal means in the infinite limits:

\[
\mathbb{E}[f(a)] = \lim_{|\mathcal{E}| \to \infty} \mathbb{E}[\hat{f}(a)] \tag{3.5}
\]

\[
\langle f_r \rangle_a = \lim_{b \to \infty} \hat{f}_r \tag{3.6}
\]

The autocorrelation function \( R^{TS}_{yy}(\Delta t) \)
\[ R_{yy}^{TS}(\Delta t) \equiv E[y(t)y(t + \Delta t)] \tag{3.7} \]
defined on the domain \( \Delta t \in \mathbb{R} \) and is symmetric about \( \Delta t = 0 \) due to the assumption of wide-sense stationarity, explained below. The same information can be captured in a one-sided autocorrelation function \( R_{yy}^{OS}(\Delta t) \), defined
\[ R_{yy}^{OS}(\Delta t) \equiv 2R_{yy}^{TS}(\Delta t), \text{ for } \Delta t \geq 0 \tag{3.8} \]
In general, one-sided quantities are preferred, so \( R_{yy}(\Delta t) \) is used to refer to \( R_{yy}^{OS}(\Delta t) \).
\( R_{yy}(\Delta t) \) captures the time-correlations of \( y(t) \) over the whole ensemble \( \mathcal{E} \). By contrast, the time-average autocorrelation function is defined for a single run \( r \)
\[ \mathcal{R}_{yy}(\Delta t, r) \equiv 2 \langle y_r(t)y_r(t + \Delta t) \rangle_t, \text{ for } \Delta t \geq 0 \tag{3.9} \]
where \( \mathcal{R}_{yy}(\Delta t, r) \) is directly defined to be one-sided. Care should be taken to distinguish these two autocorrelation quantities, as \( \mathcal{R}_{yy}(\Delta t, r) \) is often used to estimate \( R_{yy}(\Delta t) \), via the assumption of ergodicity, which is defined below.

The following assumptions are made about \( y(t) \):
- that it is a continuous-time real-valued stochastic process
- that it is defined on \( t \in [0, \infty) \)
- that its ensemble mean is zero at every instant: \( E[y(t)] = 0, \forall t \) and for \( |\mathcal{E}| \to \infty \)
- that its probability density function (PDF) is Gaussian, i.e. that \( \forall t, y(t) \) is distributed in a Gaussian manner over \( \mathcal{E} \)
- that it is wide-sense stationary (WSS), i.e. that its two-sided ensemble autocorrelation function \( R_{yy}^{TS}(\Delta t) \) is invariant under time-translations of \( \Delta t \)

An important concept concerning the relationship between time and ensemble properties of a process \( f(a) \) is ergodicity. Broadly speaking, an ergodic process is one whose ensemble averages can be found via the time averages of a particular realisation of that process. The two relevant cases of ergodicity are: ergodicity in the mean and ergodicity in the autocorrelation:
\[ \langle f_r \rangle_a = E[f(a)] \tag{3.10} \]
\[ \mathcal{R}_{ff}(\Delta t, r) = R_{ff}(\Delta t) \tag{3.11} \]
for all \( r \). For practical purposes, ergodicity may be assumed in order to justify the use of a time-average quantity as an estimator of an ensemble average, which may be difficult to calculate independently. In the context of real experiments, it is not usually possible to simultaneously measure an ensemble of identical systems. Instead, the measurements are repeated and their outcomes combined to provide an estimate of ensemble quantities. In these instances, the validity of the estimate depends on whether the process is properly ergodic.
3.2 Power spectral density

Many experimental devices, such as spectrum analysers, work natively in the frequency domain. It is therefore useful to describe characteristics of the noise as a power spectral density (PSD). The PSD of $y(t)$ is found via its one-sided truncated Fourier transform, denoted $Y_T(\omega)$, which is defined

$$Y_T(\omega) \equiv \int_0^T y(t)e^{-i\omega t}dt$$  (3.12)

using the angular frequency, non-unitary convention for Fourier transform that is common in physics. The truncated Fourier transform is used here because there is no guarantee that the integral of $y_r(t)$ for a single run will converge over $t \in [0, \infty)$. The tactic is to place a finite upper bound $T$ on the integral, take the expectation value and then take the limit $T \to \infty$.

The PSD of $y(t)$, written $S_{yy}(\omega)$, is thus defined

$$S_{TT}^{SS}(\omega) \equiv \lim_{T \to \infty} \frac{E[|Y_T(\omega)|^2]}{T}$$  (3.13)

By this definition, $S_{yy}(\omega)$ is a non-negative even function whose domain is all real $\omega$, and is hence known as a two-sided PSD. The corresponding one-sided PSD can be found in a straightforward way:

$$S_{yy}^{OS}(\omega) = 2S_{yy}^{TS}(\omega), \text{ for } \omega \geq 0$$  (3.14)

Since one-sided PSDs are more convenient and more commonly used, PSDs without the superscripts $OS$ or $TS$ are understood to refer to the one-sided version, by analogy with the autocorrelation function, hence

$$S_{yy}(\omega) \equiv 2 \lim_{T \to \infty} \frac{E[|Y_T(\omega)|^2]}{T}, \text{ for } \omega \geq 0$$  (3.15)

The definitions for autocorrelation functions and PSD can be generalised to involve two separate WSS processes $x(t)$ and $y(t)$:

$$R_{xy}(\Delta t) \equiv 2 E[x(t)y(t + \Delta t)]$$  (3.16)
$$R_{\hat{x}y}(\Delta t) \equiv 2 \langle x(t)y(t + \Delta t) \rangle_t$$  (3.17)
$$S_{xy}(\omega) \equiv 2 \lim_{T \to \infty} \frac{E[X_T^*(\omega)Y_T(\omega)]}{T}$$  (3.18)

all of which are defined to be one-sided, i.e. over $\Delta t \in [0, \infty)$ and $\omega \in [0, \infty)$. These quantities are referred to as cross-correlation functions and cross-power spectral densities.

3.3 The Wiener-Khinchin theorem

This theorem is the mathematical basis on which it is possible to describe in the frequency domain the effect of a measurement and control protocol, in the presence of noise. This theorem states that, under special conditions, the two-sided PSD $S_{ff}^{TS}(\omega)$ and the two-sided autocorrelation function $R_{ff}^{TS}(\Delta t)$
of the function \(f(a)\) form a Fourier pair \([80]\). Some of these special conditions are:

- that \(f(a)\) is WSS
- that \(R_{ff}^{TS}(\Delta t)\) exists and is finite for all \(\Delta t\)
- that the integrated spectrum \(F(\omega) \equiv \int_0^\omega S_{ff}^{TS}(\omega')d\omega'\) is continuous and differentiable everywhere
- that \(S_{ff}^{TS}(\omega)\) and \(R_{ff}^{TS}(\Delta t)\) satisfy the conditions for Fourier inversion to be valid

This section proves the theorem for the case of \(y(t)\) as defined here. Substituting the definition of \(Y_T(\omega)\) (3.12) into the definition of the PSD (3.15) gives

\[
S_{yy}^{TS}(\omega) = \lim_{T \to \infty} \frac{1}{T} \mathbb{E} \left[ \int_0^T y^*(t)e^{i\omega t} dt \int_0^T y(t')e^{-i\omega t'} dt' \right] \quad (3.19)
\]

\[
= \lim_{T \to \infty} \frac{1}{T} \int_0^T \int_0^T \mathbb{E}[y(t)y(t')]e^{i\omega(t-t')} dt dt' \quad (3.20)
\]

\[
= \lim_{T \to \infty} \frac{1}{T} \int_0^T \int_0^T \mathbb{E}[y(t)y(t+\Delta t)]e^{-i\omega\Delta t} dt dt' \quad (3.21)
\]

\[
= \lim_{T \to \infty} \frac{1}{T} \int_0^T \int_0^T R_{yy}^{TS}(\Delta t)e^{-i\omega\Delta t} dt dt' \quad (3.22)
\]

where \(y^*(t)\) denotes the complex conjugate of \(y(t)\) (since \(y(t)\) is real, \(y^*(t) = y(t)\)) and the substitution \(t' = t + \Delta t\) is made. In order to convert the double integral in \(dt\) and \(dt'\) into a single integral in \(d\Delta t\), the geometrical argument in \([56]\) is used to write

\[
S_{yy}(\omega) = \lim_{T \to \infty} \frac{1}{T} \int_{-T}^T (T - \Delta t)R_{yy}^{TS}(\Delta t)e^{-i\omega\Delta t} d\Delta t \quad (3.23)
\]

\[
= \int_{-\infty}^\infty R_{yy}^{TS}(\Delta t)e^{-i\omega\Delta t} d\Delta t \quad (3.24)
\]

\[
= \mathcal{F}\{R_{yy}^{TS}(\Delta t)\} \quad (3.25)
\]

where \(\mathcal{F}\{x(t)\}\) denotes the two-sided Fourier transform of \(x(t)\).

By substituting the relation between the one- and two-sided PSD (3.14), it is possible to derive the same result for the one-sided quantities, i.e. \(S_{yy}^{OS}(\omega) = \mathcal{F}\{R_{yy}^{OS}(\Delta t)\}\). This result is valid provided

\[
\int_{-\infty}^\infty \Delta t R_{yy}(\Delta t)e^{-i\omega\Delta t} d\Delta t < \infty \quad (3.26)
\]

This Fourier pair relationship also holds between the cross-correlation function and the cross-PSD for two different signals \(x(t)\) and \(y(t)\):

\[
R_{xy}(\Delta t) \xleftarrow{\text{FT}} \xrightarrow{\text{IFT}} S_{xy}(\omega) \quad (3.27)
\]

For non-WSS processes, a more general proof is required than is given here. Some sources use this result in order to define the PSD in terms of the autocorrelation function \([2, 14, 5, 66]\).

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Chapter 4

Characterising the Fidelity of Qubit Control

4.1 Introduction to quantum control

A primary requirement for precision quantum control is the suppression of qubit error due to environmental noise, which allows the coherence of the quantum state to be maintained [24]. In the field of quantum control, dynamical error suppression (DES) is an open-loop control technique that allows for the possibility long-term quantum memories [42] and high-accuracy single-qubit logic gates [25]. The filter transfer function approach, which frames the task of DES as a filter-design problem [6], is applied in this chapter to arbitrary, single-qubit control. Analytic expressions are derived for control fidelity in the presence of universal noise.

This chapter and the following chapter presents the work published as [69] and reproduced in Appendix A. This chapter focusses on the theoretical underpinning of qubit control, and is organised as follows. Section 4.2 presents an average Hamiltonian theory for deriving expressions for fidelity, which quantifies the effect of stochastic noise on a qubit under universal control. Section 4.3 presents a Magnus expansion of the fidelity in order to express it in the convenient overlap integral form that is easily utilised in experiment.

4.2 Fidelity metric for effect of noise on qubit control

With a spectral model for the noise affecting the qubit, it is necessary to determine the effect of that noise on the accuracy of the qubit control operation. Uncompensated stochastic noise during control operations, e.g. quantum logic gates, results in errors in the qubit evolution. The suppression of such noise is vital to applications such as quantum error correction (QEC), which require very low error rates and detailed understanding of the noise processes causing those errors [59].

The metric used to quantify the deleterious effect of noise is the average fidelity of the desired operation on the qubit state, i.e. a measure of how accurately that operation is performed in the presence of noise. This fidelity is a proxy for the coherence of the quantum state at the end of the pulse. To capture the evolution of the qubit state in the presence of universal (i.e. both dephasing and amplitude) stochastic noise, as well as coherently driven control, an average Hamiltonian theory is employed. The qubit evolution can be modelled as unitary in this experiment because: (i) there are no projective measurements made during this open-loop control protocol, and (ii) the dynamics are non-dissipative on the timescale of the experiment [69].

The main theoretical challenge is that the universality of the noise and control means that the qubit’s Hamiltonian does not necessarily commute with itself at different times, which severely complicates the analytic expression. The problem is simplified by using a Magnus expansion of the quantum state propagator $\tilde{U}(\tau)$, where the nested commutators appear only in high-order terms that may be truncated in the weak noise limit [24]. The work of Green et al. [25, 24] forms the core theoretical framework of this chapter.
4.2.1 Single-qubit Hamiltonian picture

The derivation begins with the single qubit state, which is used to represent the state of an ensemble of identical non-interacting qubits such as an ion cloud

\[ |\psi\rangle = \cos(\theta/2) |0\rangle + \sin(\theta/2)e^{i\phi} |1\rangle \]  

(4.1)

where \( \theta \) and \( \phi \) are the polar and azimuthal angles of the Bloch vector representing the state. Since the qubit experiences only unitary evolution due to both noise and control, it obeys the Schrödinger equation

\[ i\frac{d}{dt} \hat{U}(t, 0) = \hat{H}(t) \hat{U}(t, 0) \]  

(4.2)

where \( \hbar = 1 \), \( \hat{H}(t) \) is the time-dependent Hamiltonian experienced by the qubit and \( \hat{U}(t, 0) \) is the propagator that captures the time evolution of the state: \( |\psi(t)\rangle = \hat{U}(t, 0)|\psi(0)\rangle \) for \( t \geq 0 \). For convenience the initial time argument may be assumed to be 0 and dropped: \( \hat{U}(t) \)

The overall Hamiltonian can be separated into parts pertaining to the noise and to the control

\[ \hat{H}(t) = \hat{H}_N(t) + \hat{H}_C(t) \]  

(4.3)

where

\[ \hat{H}_N(t) = b(t)\sigma \]  

(4.4)

\[ \hat{H}_C(t) = h(t)\sigma \]  

(4.5)

where \( b(t) = [b_x(t) \ b_y(t) \ b_z(t)] \) and \( h(t) = [b_x(t) \ b_y(t) \ b_z(t)] \) are \( 1 \times 3 \) matrices of the noise and control fields respectively, while \( \sigma = [\hat{\sigma}_x \ \hat{\sigma}_y \ \hat{\sigma}_z]^T \) is a \( 3 \times 1 \) matrix of the three Pauli spin operators. Rather than attempting to solve directly for the overall Hamiltonian \( \hat{H}(t) \), a ‘control propagator’ is defined as the solution of the Schrödinger equation under \( \hat{H}_C(t) \) alone

\[ i\frac{d}{dt} \hat{U}_C(t) = \hat{H}_C(t) \hat{U}_C(t) \]  

(4.6)

In general, this equation cannot be integrated to determine the state evolution, due to non-commuting terms. It is therefore necessary to adopt another reference frame that makes calculation of the state fidelity more tractable.

To this end, an ‘error propagator’ \( \hat{U}(t) \) is defined that captures any deviation from the desired state trajectory due to noise

\[ \hat{U}(t) = \hat{U}_C(t)\hat{U}(t) \]  

(4.7)

and a ‘toggling frame Hamiltonian’ is defined

\[ \hat{H}_N(t) = \hat{U}_C^{-1}(t)\hat{H}_N(t)\hat{U}_C(t) \]  

(4.8)

This toggling frame is interpreted as the rest frame of the noiseless control at all times \( t \). By substitution it is found that the error propagator satisfied the Schrödinger equation governed by the toggling frame Hamiltonian
\[ i \frac{d}{dt} \tilde{U}(t) = \tilde{H}_N(t) \tilde{U}(t) \]  

(4.9)

The error propagator \( \tilde{U}(t) \) therefore describes the time evolution under the noise Hamiltonian alone. In the cases where there is no noise, or the noise is effectively suppressed by some control protocol, the error propagator is the identity \( \tilde{U}(t) = \hat{I} \).

By substituting the definition of the noise Hamiltonian (4.4) into that of the toggling frame Hamiltonian (4.8), it is possible to define a \( 3 \times 3 \) ‘control matrix’ \( \mathbf{T} \) [24] that captures the reorienting effect of coherent control

\[
\tilde{H}_N(t) = \sum_{i=x,y,z} \beta_i(t) \hat{U}_C^\dagger(t) \hat{\sigma}_i \hat{U}_C(t) 
\]

(4.10)

\[
\tilde{H}_N(t) = \sum_{i,j=x,y,z} \beta_i(t) T_{ij} \hat{\sigma}_j 
\]

(4.11)

\[
\beta(t) \mathbf{T}(t) \sigma 
\]

(4.12)

Since this expression is the product of a matrix with the Pauli matrices, the term \( \beta(t) \mathbf{T}(t) \) is identified with a \( 1 \times 3 \) ‘error matrix’ \( a(t) \) that captures the evolution of the Bloch vector due to noise alone (i.e. in the toggling frame), giving

\[
a(t) = \beta(t) \mathbf{T}(t) 
\]

(4.13)

4.2.2 Magnus expansion of the Hamiltonian

The presence of noncommuting operators in the Hamiltonian makes calculation of the propagator intractable, due to the exponentiation required to find the propagator \( \hat{U} \propto e^{-i\hat{H}} \). It is therefore necessary to approximate \( \hat{U} \) by employing a Magnus expansion and truncating at a useful point [53]. The Magnus expansion of the toggling frame Hamiltonian is written

\[
\tilde{H}_N(t) = \sum_{\mu=1}^{\infty} \Phi_\mu(t) 
\]

(4.14)

where the first few terms in the expansion are [24]

\[
\Phi_1 = \int_0^t \tilde{H}_N(t_1) dt_1 
\]

(4.15)

\[
\Phi_2 = -i \frac{1}{2} \int_0^t \int_0^{t_1} [\tilde{H}_N(t_1), \tilde{H}_N(t_2)] dt_2 dt_1 
\]

(4.16)

\[
\Phi_3 = -\frac{1}{6} \int_0^t \int_0^{t_1} \int_0^{t_2} [\tilde{H}_N(t_1), [\tilde{H}_N(t_2), \tilde{H}_N(t_3)]] + [\tilde{H}_N(t_3), [\tilde{H}_N(t_2), \tilde{H}_N(t_1)]] dt_3 dt_2 dt_1 
\]

(4.17)

By substituting the definition of the control matrix \( \mathbf{T}(t) \) (4.10) into the Magnus expansion, it is possible to expand the error matrix \( a(t) \):
\[ a(t) = \sum_{\mu=1}^{\infty} a_\mu = \beta(t) T(t) \]  
\[ (4.18) \]
\[ (4.19) \]

where the row matrix \( \bar{T}_i \equiv [T_{ix} T_{iy} T_{iz}] \) is defined in order to write

\[ a_1(t) = \sum_{i=x,y,z} \int_0^t \beta_i(t_1) \bar{T}_i(t_1) \, dt_1 \]  
\[ (4.20) \]
\[ a_2(t) = \sum_{i,j=x,y,z} \int_0^t \int_0^{t_1} \beta_i(t_1) \beta_j(t_2) (\bar{T}_i(t_1) \times \bar{T}_j(t_2)) \, dt_2 \, dt_1 \]  
\[ (4.21) \]
\[ a_3(t) = \frac{2}{3} \sum_{i,j,k=x,y,z} \int_0^t \int_0^{t_1} \int_0^{t_2} \beta_i(t_1) \beta_j(t_2) \beta_j(t_3) \]  
\[ (\bar{T}_i(t_1) \times (\bar{T}_j(t_2) \times \bar{T}_k(t_3))) + (\bar{T}_k(t_3) \times \bar{T}_j(t_2)) \times \bar{T}_i(t_1)) \, dt_3 \, dt_2 \, dt_1 \]  
\[ (4.22) \]

The commutators in the above are converted into cross products using the identity

\[ [u\sigma, v\sigma] = 2i(u \times v)\sigma \]  
\[ (4.23) \]

for all \( u, v \) with real elements [24].

The Magnus expansion has traditionally been used as a perturbative tool to deal with static errors, such as those that arise from spatial inhomogeneities in NMR ensembles [81]. This treatment applies the Magnus expansion to the control matrix \( T \), which captures the time variations of the noise, producing two distinct sets of orders of terms: the Magnus order and the filter order. This distinction does not arise in the traditional NMR case because the time invariance of the inhomogeneities cancels all the high filter order terms, leaving Magnus order as the only meaningful expansion. In the next chapter, the distinction between Magnus and filter order is elaborated and demonstrated experimentally. A recent mathematical proof of the distinction between Magnus and filter order is given in [63].

### 4.3 Fidelity metric for control accuracy

#### 4.3.1 Magnus expansion of fidelity

A useful metric for quantifying the extent to which a propagator \( \hat{U}_1 \) replicates a desired propagator \( \hat{U}_2 \), hence acting as a proxy for the accuracy of an operator in the presence of noise, is the **trace fidelity**

\[ \mathcal{F}(t) \equiv \frac{1}{4} \left| \text{Tr}[\hat{U}_2^T \hat{U}_1] \right|^2 \]  
\[ (4.24) \]

In experimental settings, the figure of merit is the ensemble average of the fidelity \( \text{E}[\mathcal{F}(t)] \). In the above formalism, the desired propagator is always \( \hat{I} \) in the toggling frame, while the actual propagator enacted is \( \hat{U}(t) \), so the average fidelity is given by

\[ \text{E}[F(t)] = \frac{1}{4} \text{E} \left[ \left| \text{Tr}[\hat{U}(t)] \right|^2 \right] \]  
\[ (4.25) \]
Expressing the error propagator in terms of the error vector, the average fidelity may be written

$$E[F] = \frac{1}{2}(E[\cos(2a)] + 1)$$  \hspace{1cm} (4.26)

where $a = |a|$ is the magnitude of the error vector and the explicit time-domain dependence of $F$ has been suppressed. Expanding the cosine term in a power series gives

$$E[F] = \left(1 - E[a^2] + \frac{2}{3}E[a^4] - \cdots\right)$$  \hspace{1cm} (4.27)

and then Magnus expanding $E[a^2]$

$$E[a^2] = \sum_{\mu,\nu=1}^{\infty} E[a_\mu a_T^{\nu}]$$  \hspace{1cm} (4.28)

$$= E[a_1]^2 + E[a_2]^2 + \cdots + 2(E[a_1 a_2^T] + E[a_1 a_3^T] + E[a_2 a_3^T] + \cdots)$$  \hspace{1cm} (4.29)

as well as the more complicated quartic term $E[a^4]$ gives, with rearrangement in terms of Magnus order,

$$E[F] = 1 - E[a_1^2] - 2E[a_1 a_2^T] - \left(E[a_2^2] + 2E[a_1 a_3^T] - \frac{a_1^4}{3}\right) + \cdots$$  \hspace{1cm} (4.30)

These terms can be expressed in terms of auto- and cross-correlation functions as described in section 3.2: the $a_1$ terms contain two-point correlation functions, the $a_2$ terms contain four-point correlation functions, and so on. For sufficiently weak noise, the quadratic term of $a_1$ is the dominant contributor to fidelity and all higher powers of $a_1$ may be neglected, as well as the higher Magnus orders $a_2, a_3, \cdots$. [24]. The truncated first-order average fidelity is thus written

$$E[F_1] = 1 - E[a_1^2]$$  \hspace{1cm} (4.31)

### 4.3.2 Fidelity approximations beyond the quadratic power

The criterion for ‘sufficiently weak noise’ used to justify truncating the power series (4.30) at the quadratic term is given by a smallness parameter

$$\xi \equiv \Delta y \tau / 2$$  \hspace{1cm} (4.32)

where $\Delta y = \sqrt{E[y^2]}$ is the root-mean-square (RMS) of the noise and $\tau$ is the total time duration of the control protocol [25]. The quadratic truncation is used in situations where $\xi^2 \ll 1$. In cases where the noise too strong for this criterion to be fulfilled, the first-order average fidelity $E[F_1]$ ceases to be a useful metric [69]. It becomes necessary to include higher powers of the first-order Magnus order term $E[a_1^{2m}]$ for $m > 1$. The similarity between the higher powers of $E[a_1^2]$ and the power series expansion of the exponential $e^{2E[a_1^2]}$ allows for the definition of a new fidelity expression $E[F_\chi]$ where

$$E[F_\chi] = \frac{1}{2} \left( 1 + e^{-\chi(t)} \right)$$  \hspace{1cm} (4.33)

$$= 1 - E[a_1^2] + E[a_1^4] - \frac{2E[a_1^6]}{3} + \cdots$$  \hspace{1cm} (4.34)

$$\approx E[F]$$  \hspace{1cm} (4.35)
where the error is $\chi(t) = E[a_1^2]$, as above. The distinctions between the three average fidelity quantities are:

- $E[\mathcal{F}]$ includes all powers of all Magnus terms, valid for all $\xi$
- $E[\mathcal{F}_1]$ includes the quadratic power of first Magnus term, valid for $\xi^2 \ll 1$
- $E[\mathcal{F}_\chi]$ includes all powers of first Magnus term, valid for $\xi^2 \lesssim 1$ (though agreement with experiment is shown even for $\xi^2 = 1$ [69])

Since $E[\mathcal{F}_\chi]$ is useful for a wider range of noise strengths but still has a simple exponential form that is expressible in terms of $a_1$ alone, it is the metric of choice in the following experiments. The higher powers $E[\mathcal{F}_\chi]$ continue to dominate the higher Magnus order terms for sufficiently weak noise, which justifies disregarding contributions by $a_2, a_3, \cdots$ [69].

4.3.3 Fidelity in the frequency domain

All of the average fidelity quantities so far have been expressed in the time domain. Since it is more experimentally convenient to deal with the spectral characteristics of stochastic noise processes, it is desirable to translate the problem into the frequency domain. The derivation begins by finding the overlap integral for $E[\mathcal{F}_1]$, which contains only two-point correlation functions of the form $R_{ij}(t_1, t_2)$. The higher Magnus terms $a_\mu$ for $\mu > 1$ that contribute to $E[\mathcal{F}]$ contain $n$-point functions $R_{ij}^{(n)}(t_1, \cdots, t_n)$ (for even $n$ only), but since $y(t)$ is assumed to be Gaussian-distributed, the Gaussian moment theorem can be applied to express the $n$-point correlation functions in terms of two-point correlation functions [25, 24]. Hence the substitution $E[\mathcal{F}_1] \rightarrow E[\mathcal{F}]$ is done after the conversion to the frequency domain by defining higher-power filter functions $F^{(n)}(\omega, \cdots)$ to include contributions from the $n$-point correlations.

The time-domain expression for the truncated first-order average error is written

$$E[a_1^2] = \sum_{i,j=x,y,z} \int_0^t \int_0^t E[\beta_i(t_1)\beta_j(t_2)] \bar{T}_i(t_1)\bar{T}_j^T(t_2) dt_2 dt_1$$

(4.36)

$$= \sum_{i,j=x,y,z} \int_0^t \int_0^t R_{ij}^{TS}(t_1, t_2) \bar{T}_i(t_1)\bar{T}_j^T(t_2) dt_2 dt_1$$

(4.37)

$$= \sum_{i,j=x,y,z} \int_0^t \int_0^t R_{ij}^{TS}(t_2 - t_1) \bar{T}_i(t_1)\bar{T}_j^T(t_2) dt_2 dt_1$$

(4.38)

where $R_{ij}^{TS}(t_1, t_2)$ is the two-sided cross-correlation function derived in the previous section, and the third line is valid assuming all the noise processes are WSS.

Using the Wiener-Khinchin theorem derived in section 3.3, it is possible to use the PSD of the noise

$$R_{ij}(t_2 - t_1) = \frac{1}{2\pi} \int_{-\infty}^{\infty} S_{ij}(\omega) e^{i\omega(t_2 - t_1)}$$

(4.39)

as well as Fourier transforming the control matrix elements

$$T_{ij}(\omega) = \int_0^t T_{ij}(t_1)e^{-i\omega t_1} dt_1$$

(4.40)

to obtain the overlap integral for the first-order average fidelity.
\[E[F_1] = 1 - \frac{1}{2\pi} \sum_{i,j=x,y,z} \int_{-\infty}^{\infty} S_{ij}(\omega) T_i(\omega) \overline{T}_j(\omega) d\omega \quad (4.41)\]

To exemplify the form of \( T(\omega) \) in experimentally-relevant situations, it can be shown [24] that for a driven rotation on the Bloch sphere around the \( X \) axis of magnitude \( \pi \), in the presence of purely dephasing noise \( (\text{i.e.} \text{ where the noise vector } \vec{\beta}(t) \text{ has only a } Z\text{-component}) \), the control matrix contains only two nonzero elements:

\[
T_{zz}(\omega) = \frac{\omega^2}{\omega^2 - \Omega^2}(e^{i\omega \tau_\Omega} + 1) \quad (4.42)
\]

\[
T_{zy}(\omega) = \frac{i\omega \Omega}{\omega^2 - \Omega^2}(e^{i\omega \tau_\Omega} + 1) \quad (4.43)
\]

where \( \Omega = \pi/\tau_\Omega \) is the Rabi rate of the coherent driving of the qubit.

The frequency-domain control matrix \( T(\omega) \) provides the elements for calculating the filter transfer functions known in the quantum dynamical error suppression (DES) literature [6, 24]. The primary difference between the above derivation and those found in the DES literature is in the definition of (4.40), where the literature includes a factor of \(-i\omega\) in the righthand side of the definition. By omitting this factor, the thesis uses a consistent definition that is valid for both the ‘filter functions’ known to the DES community and the ‘transfer functions’ known to the frequency metrology community. The two functions are mathematically identical and in this treatment are defined in the same way.

A simple and experimentally-useful example of deriving a filter function from the control matrix is the case of pure dephasing noise [25]. The error due to dephasing \( \chi_z \) is given to first Magnus order by

\[
\chi_z = \frac{1}{2\pi} \int_{-\infty}^{\infty} S_z(\omega) F_z^{(1)}(\omega) d\omega \quad (4.44)
\]

where the fidelity is reduced by dephasing alone \( E[F_1] \simeq 1 - \chi_z \) and the first-Magnus-order, dephasing filter function is defined

\[
F_z^{(1)}(\omega) \equiv \sum_{i=x,y,z} |T_{zi}(\omega)|^2 \quad (4.45)
\]

Another important source of noise in experimental systems is amplitude noise, which is coaxial with the driving field. Since the axis of noise varies as the direction of driven control of the qubit, it is necessary to define the time-dependent axis of rotation \( \vec{\sigma}_\Omega = \cos (\phi(t)) \hat{\sigma}_x + \sin (\phi(t)) \hat{\sigma}_y \) of the driving field. The error due to amplitude noise has the same form

\[
\chi_\Omega = \frac{1}{2\pi} \int_{-\infty}^{\infty} S_\Omega(\omega) F_\Omega^{(1)}(\omega) d\omega \quad (4.46)
\]

where the first-Magnus-order amplitude filter function is defined

\[
F_\Omega^{(1)}(\omega) \equiv \sum_{i=x,y,z} \cos^2 (\phi(t)) |T_{xi}(\omega)|^2 + \sin^2 (\phi(t)) |T_{yi}(\omega)|^2 \quad (4.47)
\]

In the presence of universal noise, the contributions from dephasing and amplitude noise are simply summed
$$E[\mathcal{F}_1] = 1 - (\chi_z + \chi_\Omega) \quad (4.48)$$
$$= 1 - \frac{1}{2\pi} \int_{-\infty}^{\infty} (S_z(\omega) F_z^{(1)}(\omega) + S_\Omega(\omega) F_\Omega^{(1)}(\omega)) \, d\omega \quad (4.49)$$

A replacement of the truncated first-order average fidelity $E[\mathcal{F}_1]$ with the preferred $E[\mathcal{F}_\chi]$ requires only a substitution of the term $E[a_1^2]$ by the exponential $e^{-2E[a_1^2]}$, as indicated by the definition (4.33)

$$E[\mathcal{F}_\chi] = \frac{1}{2} \left( 1 + e^{-\chi(t)} \right) \quad (4.50)$$
$$= \frac{1}{2} \left( 1 + \exp \left[ \frac{1}{2\pi} \sum_{i=z,\Omega} \int_{-\infty}^{\infty} S_i(\omega) F_i^{(1)}(\omega) \, d\omega \right] \right) \quad (4.51)$$

It is important to note that this expression contains only first-order Magnus contributions.

To calculate the full unapproximated average fidelity $E[F]$ requires the inclusion of high-order Magnus terms, which therefore involve the use of $n$-order filter functions:

$$E[\mathcal{F}] = 1 - \frac{1}{2\pi} \sum_{i=z,\Omega} \int_{-\infty}^{\infty} S_i(\omega) F_i^{(1)}(\omega) \, d\omega + \frac{1}{(2\pi)^2} \sum_{i=z,\Omega} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} S_i(\omega) S_i(\omega') F_i^{(2)}(\omega, \omega') \, d\omega \, d\omega' + \cdots \quad (4.52)$$

where the Gaussian moment theorem has allowed the $n$-point noise correlations $R_{ij}(t_1, t_2, \cdots, t_n)$ to be Fourier transformed into powers of the two-point quantity $S(\omega)$ [25]. Hence the only new quantities required are the higher order filter functions $F^{(n)}(\omega, \cdots)$. A more generalised approach for calculating the higher order filter functions in terms of a set of fundamental filter functions has been recently derived in [63].

The next chapter will test and verify the accuracy of this overlap integral expression for $E[\mathcal{F}_\chi]$ as a metric for experimentally measured qubit fidelity. Using insights from the spectral analysis of this framework, existing composite pulse schemes for error suppression are extended and improved, leading to a new understanding of the practical benefits of using the filter function in this way.
Chapter 5

The Filter Function Approach to Characterising Qubit Control

5.1 Introduction to composite pulse methods of quantum control

This chapter presents the first experimental validation of generalised filter-transfer functions casting arbitrary quantum control operations as noise spectral filters [25, 24]. Using this validated theoretical framework, composite pulses known from the magnetic resonance community are analysed and experimentally tested. The filter function framework plays a central role in both characterising and improving the performance of traditional and novel composite pulse schemes.

The use of composite pulses for noise suppression in quantum systems has received significant attention [11, 43, 4]. Many open-loop quantum control techniques make use of ideas from nuclear magnetic resonance (NMR) due to the structural similarities between the qubit architecture and the spin-ensemble system [6, 4], while others have been developed as Hamiltonian-engineering approaches for quantum computation [43, 41]. Using a framework known as *Walsh basis synthesis* to systematise and unify the methods for constructing composite pulses, this chapter demonstrates these pulses’ enhanced error-suppressing properties in comparison to non-compensated ‘primitive’ pulses. The experimental results also contribute to the characterisation of these pulses, by demonstrating the utility of the filter function description in realistic, time-varying noise environments.

This chapter and the previous chapter presents the work published as [69] and is organised as follows. Section 5.2 outlines the experimental setup specific to the qubit control experiment. Section 5.3 presents results showing the predictive power of fidelity calculations based on filter functions, in the case of ‘primitive’ uncorrected pulses. Section 5.4 introduces the composite pulses sequences of interest: BB1 (broadband) and SK1 (Solovay-Kitaev). It also demonstrates the conceptual distinction between Magnus order and filter order in determining fidelity, by means of an experimental single-tone spectral scan. Section 5.5 presents results demonstrating the improved noise filtering capability of amplitude-modulated pulses synthesised using higher-order Walsh functions, which systematises previous work done on dynamically-corrected gates (DCG) [43].

5.2 Quantum control experiment setup

The experiment involves the application of composite microwave pulses to a trapped ion cloud, with a user-defined noise spectrum engineered on the microwave carrier, and the measurement of the pulse fidelity via photon counts. The trapping and optical setup described in Chapter 2 is common to this experiment and the frequency standard experiment. The only features specific to the composite pulse experiment are: (i) the IQ modulation for engineering noise on a continuously-driven pulse, and (ii) the software for synthesising pulses in the Walsh basis.
5.2.1 Noise engineering

This thesis is concerned with demonstrating techniques for precision control in the presence of arbitrary noise power spectral densities (PSD). It is therefore necessary to emulate a variety of noise environments by deliberately degrading the microwave signal according to a user-determined noise PSD. This deliberate error is scaled to completely dominate the effect of ‘intrinsic’ phase and amplitude noise in the microwaves, so that the ‘engineered’ noise PSD of the output microwaves accurately reflects the desired noise character.

While $S_{yy}(\omega)$ can in general be any positive semi-definite function of $\omega$, the standard model for noise PSDs relevant to both the composite pulse and frequency standard experiments is the power law model. This model expresses the PSD as the sum of powers of $\omega$ such that particular power-dependences dominate in particular regions. In these experiments, a power-law model defined on three regions is used, whose boundaries are defined by the low roll-off frequency $\omega_b$ and the high roll-off frequency $\omega_c$:

$$S_{yy}(\omega) = \begin{cases} r_b(\omega), & \text{for } \omega < \omega_b \\ \sum_{n=-2}^{+2} h_n \omega^n, & \text{for } \omega \in [\omega_b, \omega_c] \\ r_c(\omega), & \text{for } \omega > \omega_c \end{cases} \quad (5.1)$$

where $r_b(\omega)$ and $r_c(\omega)$ are the two roll-off functions that describe the PSD behaviour for very low and very high frequencies, and the coefficients are set to ensure $S_{yy}(\omega)$ is continuous over the whole domain. In these experiments $r_b(\omega)$ is often set to a constant (‘white ceiling’) and $r_c(\omega)$ to 0 (‘hard cutoff’), although the model gives extensive scope for customising the PSD to mimic realistic noise settings.

In the relevant physical settings, phase and amplitude errors arise by different noise processes, and so the engineered noise in each of these quadratures is synthesised separately. As seen in the previous chapter, a range of noise processes including qubit dephasing due to environmental interactions, as well as phase and amplitude errors in the driving microwave field, may be emulated by performing amplitude and phase modulation (AM and PM) on the driving field only [70]. Since the engineered noise PSD is expressed in the frequency domain, a Fourier transform is required to obtain the time-domain AM and PM waveforms. The noisy control field may be written

$$B(t) = \Omega (1 + \beta_\Omega(t)) \cos (\omega t + \beta_\Phi(t)) \hat{n} \quad (5.2)$$

where $\beta_\Omega,\Phi(t)$ are the AM and PM waveforms, $\Omega$ and $\omega$ are the carrier amplitude and frequency, and $\hat{n}$ is the spatial direction of the magnetic part of the control field. The modulating waveforms are expanded as a discrete truncated inverse Fourier transform

$$\beta_\Omega(t) = \alpha_\Omega \sum_{j=1}^{j_c} F_{\Omega}(j) \cos (\omega_j t + \psi_j) \quad (5.3)$$

$$\beta_\Phi(t) = \alpha_\Phi \sum_{k=1}^{k_c} F_{\Phi}(k) \cos (\omega_k t + \psi_k) \quad (5.4)$$

where $F_{\Omega,\Phi}$ are the envelope functions of the discrete PSDs, $\omega_{j,k}$ are the component frequencies, $\alpha$ is the overall noise scaling, the subscript $c$ denotes the maximum index before the high-frequency truncation, and $\psi_{j,k} \in [0, 2\pi)$ are uniformly-distributed pseudorandom phases. The desired time-correlations in the noise are captured by the envelope functions while the stochastic time-domain
Angular Frequency, $\omega$

**Figure 5.1**: A logarithmic plot of an engineered comb spectrum PSD. The envelope function $F(j)$ sets the power law behaviour, up to a hard cutoff at $J\omega_0$. Since the comb spacing is linear, it appears to become denser as frequency increases on this logarithmic plot.

behaviour is provided by the random phases between each frequency component. The spacing of $\omega_j = j\omega_0$ is linear with minimum frequency spacing $\omega_0$. The characteristic time scale of the modulating waveforms $\beta_\Omega(t)$ and $\beta_\Phi(t)$ is generally much longer than the carrier period, so $j\omega_0 \ll \omega$. When there is more than one component frequency, the discrete spectrum is referred to as a ‘comb’ spectrum, and in the limit of a single component frequency, it is referred to as a ‘tone’ spectrum. A schematic diagram of a comb spectrum is shown in Figure 5.1.

For phase errors, the *frequency* noise PSD $S_z(\omega)$ is more commonly quoted than the phase noise PSD, in which case the appropriate envelope functions are

$$F(j) = \begin{cases} j^{\frac{p}{2}} & \text{for amplitude noise} \\ j^{\frac{p}{2} - 1} & \text{for phase noise} \end{cases} \quad (5.5)$$

By setting the parameters and envelope functions in equations (5.3) and (5.4), the experimentalist is able to engineer analytic functions of stochastic noise with the desired PSD [70]. During a run of the experiment, a noise trace is generated and discretised according to the cycle structure of the particular experiment. The resulting noise samples are imposed on the microwave carrier signal, by IQM in the qubit control experiment and by FM in the frequency standard experiment.

### 5.2.2 Experimental implementation via IQ modulation

In order to drive arbitrary qubit rotations and to apply engineered noise, precise time-dependent control over the microwave phase and amplitude is necessary. The composite pulse experiment uses internal IQ modulation (IQM), according to a software-defined waveform downloaded from the experiment PC. The principle of IQM is a decomposition of the signal into in-phase (I) and quadrature (Q) components, which effectively converts combined phase and amplitude modulation of the carrier into amplitude-only modulation of the components. This can be understood as a change of basis of the signal phasor diagram from polar coordinates (amplitude and phase) to rectilinear coordinates (I and Q). Considering time-dependent amplitude modulation $A(t)$ and phase modulation $\delta(t)$ of a signal with carrier angular frequency $\omega_c$

$$S(t) = A(t) \cos(\omega_c t + \delta(t)) \quad (5.6)$$

the required decomposition can be found by trigonometric identities
\[ S(t) = I(t) \cos(\omega_c t) + Q(t) \cos(\omega_c t + \pi/2) \] (5.7)

where the modulating waveforms are defined

\[ I(t) = A(t) \cos(\delta(t)) \] (5.8)
\[ Q(t) = A(t) \sin(\delta(t)) \] (5.9)

Figure 5.2 : IQ modulation circuit diagram.

Figure 5.2 depicts a circuit diagram of IQM, represented as a circuit of mixers. The VSG downloads the modulating waveforms not as continuous functions, but as a pair of discrete vectors of ‘waveform samples’. The time interval between each sample is user-defined and the VSG’s interpolation algorithm converts the downloaded waveform file into continuous functions \( I(t) \) and \( Q(t) \) for mixing. Thus the experimentalist, by generating discrete waveform files and uploading them to the VSG, can enact arbitrary rotations of the qubit for any duration longer than the inverse of the sample rate.

5.3 Experimental validation of filter function predictions

In order to demonstrate the usefulness of this filter function approach to quantum control, it is necessary to show that the theoretical expressions for fidelity accurately predict measured fidelity. Such a test is done by performing a ‘primitive’ \( \pi \) pulse, resulting in the qubit transition \( |0\rangle \rightarrow |1\rangle \) in the presence of engineered noise. The key parameters, namely the PSD scale factor \( \alpha \) and cutoff frequency \( \omega_c \), are scanned to demonstrate the frequency-dependence of fidelity. A schematic of the cutoff scan used in this section and the single-tone scan used in section 5.4.2 is shown in Figure 5.3.
Figure 5.3: Engineered noise PSDs. The white noise spectrum (blue) takes the form of a step function with a hard cutoff at $\omega_c$ and is used for the validation experiment (section 5.3). The single-tone spectrum (black) consists of a delta function whose centre frequency $\omega_t$ is scanned for the experimental testing BB1 and SK1 composite pulse performance (section 5.4.2). The overall noise strength is expressed in terms of the noise amplitude $\alpha$.

Figure 5.4: Fidelity of a primitive $\pi$ pulse in the presence of a white noise PSD of varying strength $\alpha$. The experimentally observed bright state probability (circles) match closely the theoretically calculated fidelity $E[F_\chi]$ (solid black curves) when the smallness parameter (red line) $\xi^2 \leq 1$. The smallness parameter, as defined in the previous chapter, is proportional to the total power in the noise, and therefore determines the breakdown point (dashed vertical lines) of the first-order fidelity approximation. Each experimental data point is the average of 50 different noise realisations. The dotted line at $P(|1\rangle) = 0.5$ bright state probability indicates zero fidelity, i.e. total decoherence of the qubit state.

The measurements of single-gate fidelity in the presence of a white engineered noise spectrum
are shown in Figure 5.4, overlain with filter-function-based predictions of fidelity. Measurements are conducted for a simple $\pi_X$ enacted while varying the high-frequency cutoff, $\omega_c$, of a flat-top engineered noise PSD. As the high-frequency cutoff of the noise is increased and fluctuations that are fast compared to the control ($\tau_{\pi}$) are added to the noise power spectrum, $S_s(\omega)$, errors accumulate reducing the measured fidelity. The fidelity predictions are based on a direct calculation of $F_\chi = 1 - \exp \left[ \int_0^\infty S_s(\omega) F_\chi(\omega) d\omega \right]$. These predictions fit the experimentally observed values closely, with no free parameters. The agreement breaks down only in the strongest noise environment $\alpha = 200$, where the weak-noise assumption underpinning the first-Magnus-order approximation no longer holds.

5.4 Composite pulse sequences for noise suppression

5.4.1 Traditional composite pulses

Quantum logic requires the enactment of arbitrary single-qubit rotations $\hat{U}_\phi(\theta)$, with high fidelity even in the presence of qubit or field noise. A huge variety of composite schemes have been invented in the field of NMR, which are designed to compensate for inhomogeneities in the orienting magnetic field [75, 81]. Composite pulses work by geometrically manipulating the qubit state, such that first-order sensitivity of the state to environment noise is transformed into high-Magnus-order contributions. As these high-order contributions scale with the strength of the noise, they become insignificant in the weak-noise quasistatic limit. It has been shown that such pulses also provide significant benefits in the presence of time-varying noise, which motivates their investigation in this quantum system [11].

Two composite pulse schemes for enacting arbitrary rotations, BB1 and SK1, are constructed by performing a rotation of arbitrary angle $\theta$ on the Bloch sphere and then a series of ‘compensating’ pulses that sum to the identity operator. The net result of this composite pulse is a driven rotation of $\theta$ with higher fidelity than if the same rotation had been performed ‘primitively’, i.e. without additional error-compensating pulses. The pulses can be defined in terms of time evolution operators $\hat{U}_\phi(\theta)$ where $\phi$ is the axis of rotation on the Bloch sphere ($\phi = 0$ corresponding to $\hat{\sigma}_x$) and $\theta$ is the angle of driven rotation. The composite pulses of interest are defined

$$U^{(BB1)}_\phi(\theta) = U_{\phi + \phi_{BB1}}(\pi) U_{\phi + 3\phi_{BB1}}(2\pi) U_{\phi + \phi_{BB1}}(\pi) U_\phi(\theta)$$  \hspace{1cm} (5.10)$$

$$U^{(SK1)}_\phi(\theta) = U_{\phi - \phi_{SK1}}(2\pi) U_{\phi + \phi_{SK1}}(2\pi) U_\phi(\theta)$$  \hspace{1cm} (5.11)$$

where $\phi_{BB1} = \phi_{SK1} = \cos^{-1}(-\theta/4\pi)$ [81, 11].

In order to quantify the error-suppressing capabilities of these two composite pulse schemes, the average fidelity $E[\mathcal{F}]$ is used. It can be shown [69] that the Magnus expansion of $E[\mathcal{F}]$ for BB1 has a second-order squared leading term $E[a_2^2]$ while for SK1 the leading term is first-order squared $E[a_1^2]$. For static amplitude noise, the leading Magnus order determines the overall error suppression. A comparison of the fidelity of experimentally enacted BB1 and SK1 pulses, for varying strength of time-varying noise, allows a determination of the threshold where the first-Magnus-order approximation $E[\mathcal{F}_X]$ ceases to be a good approximation for $E[\mathcal{F}]$.

5.4.2 Single-tone engineered noise scans for BB1 and SK1

The usefulness of the Magnus-term expression of pulse fidelity and the filter function may be illustrated by comparing the performance of different composite pulses in the presence of the same noise environment. The PSD used here is an ‘amplitude tone spectrum’, which consists of a single sinusoid component at frequency $\omega_t$ of random initial phase modulating the microwave amplitude. $\omega_t$ is swept through a range, and since the tone spectrum PSD is the delta function $S(\omega) = \delta(\omega - \omega_t)$, the first-order fidelity depends directly on the filter function.
Figure 5.5: Swept single-tone scan of first-order filter function and measured fidelity for three $\pi$ pulses: primitive, SK1 and BB1. The tone angular frequency $\omega_1$ is in units of inverse $\tau_\pi$, which is the time required to enact a primitive $\pi$ rotation. (a) The solid lines indicate the first-order amplitude filter function $F_\Omega(\omega_1)$ for the three pulses. The dotted lines mark the frequencies at which the filter functions cross, indicating points of inversion in the relative performance of the pulses. (b) (weak noise) and (c) (strong noise) The solid lines indicate analytically-calculated error ($\chi_\Omega = \exp \left[ F_\Omega(\omega_1) \right]$) and markers indicate experimental measurements of error, averaged over 20 realisations of engineered noise. The physical observable used as a proxy for error is $1 - P(|1\rangle)$, since an ideal $\pi$ pulse results in $P(|1\rangle) = 1$. The noise amplitude $\alpha$ is given in terms of the driving amplitude $\Omega$. The measurement resolution limit is depicted as a grey shade.

\[
E[F_\chi] = 1 - \exp \left[ \int_0^\infty F(\omega)\delta(\omega - \omega_1)d\omega \right]
\]

\[
= 1 - \exp \left[ F(\omega_1) \right]
\]  

Single-tone scans are useful for ‘tracing out’ the shape of the filter function, indirectly observing the spectral sensitivity of a particular composite pulse sequence to noise.

A single-tone scan with varying noise strength $\alpha$ to compare a primitive $\pi$ pulse, a BB1 $\pi$ pulse and an SK1 $\pi$ pulse may be used to test the improved performance of BB1 and SK1 in contrast to the primitive pulse for time-varying noise, as well as in the static limit for which they were originally designed. Figure 5.5 shows the result of such a single-tone scan.

The vertical dotted lines indicating the filter function crossovers closely match the crossovers of experimentally measured fidelities. Hence the filter function approach accurately predicts the comparative performance of primitive, SK1 and BB1 pulses across the spectrum. In panel (b), the calculated error fits the experimental data well over three decades of frequency, down to the measurement resolution limit of $\chi < 1.5\%$, verifying the predictive power of the filter function approach in the weak noise regime. SK1 and BB1 composite pulses outperform primitive pulses in the low $\omega_1$ regime because their filter order in the quasistatic limit is quadratic, in contrast to the constant filter order of the
primitive pulse, i.e. \( F(\omega) \propto \omega^2 \) for BB1 and SK1 and \( \propto \omega^0 \) for primitive, for \( \omega \to 0 \).

In panel (e), the calculated error fits the experimental data only for frequencies higher than the primitive-SK1 crossover. In the low frequency regime, the second-order Magnus term contributes significantly to the overall fidelity and the first-order filter function ceases to accurately predict the error. The experimental fidelity \( E[\mathcal{F}] \) diverges from the calculated first-order approximation \( E[\mathcal{F}] \) differently for SK1 and BB1. As noted above, in the static limit SK1 has a first-order leading Magnus term while BB1 has a second-order leading Magnus term, i.e. there is no static, first-Magnus-order contribution to the error for BB1 as there is for SK1. This difference between the two composite pulses means that in the quasistatic regime for strong noise, the BB1 is dominated by the second order term, resulting in higher overall fidelity \( E[\mathcal{F}] \). The comparison between (b) and (c) therefore illustrates the noise strength threshold at which the filter function approach ceases to accurately predict fidelity.

The different performance of BB1 and SK1 in (e) illustrates an important theoretical result: that Magnus order and filter order are distinct and dominate the overall fidelity in different regimes. In the limit of strong, low frequency noise, the leading Magnus order provides the dominant contribution to fidelity, leading to the superior performance of BB1 over SK1 despite having the same filter order \( F_\Omega(\omega) \propto \omega^2 \). In the weak noise regime, the contribution of the first-order filter function dominates the fidelity. The distinction between Magnus and filter order that is shown experimentally in this thesis has been given a rigorous theoretical proof [63].

5.5 Search for optimised Walsh amplitude modulated filters

5.5.1 Dynamically corrected gates as composite pulses

A generalisation of the NMR approach to time-varying noise environments was proposed by Khodjasteh et al., known as ‘dynamically (error-)corrected gates’ (DCG) [43]. Such DCGs produce the same state net unitary evolution as the primitive pulses with lower error per gate, by enacting a composite pulse sequence consisting of piecewise-constant rotations about various axes. The advantages of the original dynamical correction approach are: that DCGs reduce error in a universal noise environment and that they are effective in the presence of time-varying noise governed by a stochastic Hamiltonian [41]. These features make the DCG class of composite pulses attractive for implementations in realistic physical systems, especially for the purposes of quantum logical and computation [42].

The original formulation of the DCG involves a group theoretic approach [43], but more recently it has been shown that the same pulses may be understood in terms of Walsh functions, as Walsh amplitude modulated filters [4]. The advantage of applying Walsh synthesis to the notion of DCGs is the relative ease of use of the Walsh functions, and the direct relationship between Paley order and filter order, which is demonstrated in this chapter.

5.5.2 Walsh synthesis of composite pulses

The Walsh functions, which are the square wave analogues of sine and cosine functions, provide a useful method for synthesising novel composite pulses, since they are naturally compatible with discrete-time clocking and digital logic [4]. The infinite set of Walsh functions \( \{W_k(x)\} \) are defined on the interval \( 0 \leq x \leq 1 \) and take only values \(-1\) and \(1\). The set forms an orthonormal basis and hence any continuous function may be expressed in terms of Walsh functions [78]. The number and location of zero-crossings of any Walsh function depends on its Paley order \( k \), which is the ordering convention of the Walsh set used in this work. Figure 5.6 shows plots of the first 32 Paley-ordered Walsh functions.

The formal definition of the Walsh functions is
Figure 5.6: A graphical depiction of the first 32 Paley-ordered Walsh functions. The functions of Paley order $k = 1, 3, 7, 15, 31$ are highlighted in red, as these Walsh functions have the best amplitude noise suppressing properties in their classes. A class of Walsh functions is defined as a set of Walsh functions with the same minimum inter-crossing interval. In the Paley order, each class is equivalent to a logarithmic octave in $k$.

$$W_k(x) = \prod_{j=1}^{m} \text{sgn}(\sin(2^j \pi x))^{b_j}$$

where $(b_m, b_{m-1}, \ldots, b_1)_2$ is the binary representation of $k$. The Walsh functions or superpositions of them are applied as modulation to the driving field in order to produce Walsh synthesised gates. A modulating time-domain function $M(t)$ is produced from a sum of the relevant Walsh functions

$$M(t) = \sum_{k \in S} n_k W_k(t/\tau)$$

where $S$ is the set containing the synthesised basis functions, $n_k$ is the relative scaling factor for each basis function and $\tau$ is the total duration of the whole Walsh-modulated pulse.

In the Walsh amplitude modulated filter (WAMF) pulses examined here, the value of $M(t)$ determine the strength of the applied driving field, producing piecewise-constant amplitude modulation of the driving field. It can be seen that the first-order DCG NOT gate [42] is the result of amplitude modulation by a synthesis of the zeroth and third Paley order Walsh functions

$$M_{\text{DCG}}(t) = 1.5 W_0(t/\tau) + 0.5 W_3(t/\tau)$$

with amplitude modulation depth $\Omega_R = \pi/\tau_\pi$, where $\Omega_R$ is the Rabi rate. The extension of the DCG concept to higher order is thus straightforwardly done using the Walsh functions [4].

It can be shown that other composite pulses familiar to NMR, such as BB1 and SK1, may be written in terms of Walsh-synthesised phase modulation. These two pulses consist of the initial ‘primitive’ part followed by the ‘compensating’ part, and the compensating part may be expressed in the Walsh basis:

$$M_{\text{BB1}}(t) = 2 W_0(t/\tau) + W_3(t/\tau)$$
$$M_{\text{SK1}}(t) = W_1(t/\tau)$$

with phase modulation depth $\phi_{\text{BB1}} = \phi_{\text{SK1}} = \cos^{-1}((-\theta/4\pi))$ [4].
5.5.3 Walsh synthesis software

The experiment PC runs the hardware for the composite pulse experiment using software written in the IGOR Pro language. The custom-written software module has a graphical user interface (GUI) that synthesises modulating functions $M(t)$ out of arbitrary weightings of Walsh functions, as well as standard NMR pulses such as BB1 and SK1. The engineered noise, which is expressed as a discrete ‘comb spectrum’ that approximates a continuous PSD [70], is applied by adding the engineered noisy time trace $y(t)$ to the function $M(t)$. The computer discretises these modulating functions and sends the resulting waveform vectors via GPIB link to the VSG, which then applies IQ modulation internally.

The ability to synthesise composite pulses in the Walsh basis, either by phase or amplitude modulation, makes it desirable to attempt a search for novel high-performance pulses. The Walsh basis provides a convenient restriction on the dimensionality of the search space, making the process highly efficient. The filter function formalism makes this approach particularly attractive, since the search cost function may be derived from a specific noise model or experimentally-observed PSD, which turns the search into an optimisation problem tailored to a particular need.

The cost function $A_i$ used to evaluate the performance is the integral of the filter function over a spectral band of interest $\omega \in [\omega_l, \omega_c]$, thereby capturing the bandlimited performance of a control operation:

$$A_i = \int_{\omega_l}^{\omega_c} F_i(\omega)\,d\omega \quad (5.19)$$

where $i \in [z, \Omega]$.

A convenient search space is the two-dimensional space spanned by the Walsh basis functions $W_0$ and $W_3$, to which the amplitude modulating profile for the traditional first-order DCG belongs (equation 5.16). A colour plot of the the cost function in this search space is given in Figure 5.7.

The blue regions of the colour plot correspond to areas where $A_i$ is minimised, resulting in superior error suppression. Since $W_k$ is a mean-zero function for all $k > 0$, the overall net rotation performed is given entirely by the amplitude of $W_0$. By targeting the blue regions, it is possible to easily derive an error-suppressing composite pulse for an arbitrary desired rotation $\theta = X_0 \mod 2\pi$.

The numerical search results may be verified experimentally by scanning over $X_3$ for a fixed $X_0$, shown in Figure 5.8(a)-(c). The regions of high error-suppression (blue in the colour plot), appears as infidelity troughs in the experimental data. Direct integration of the Schödinger equation in the presence of simulated noise fits the experimental data well. This data confirms that Walsh synthesis of composite pulses results in improved error suppressing for an arbitrary desired rotation $\theta$.

5.5.4 Randomised benchmarking

Randomised benchmarking [44] is used as a tool for resolving small gate errors below the measurement resolution limit. The technique works by repeating the desired pulse about a randomised axis, leading to an amplified overall error that is more easily measured, allowing the mean ‘error per gate’ to be determined. Our randomised benchmarking sequence consists of interleaved ‘reorienting’ $\pi/2$ pulses and ‘under test’ $\pi$ pulses, each applied along axes randomly selected from $\pm X$ and $\pm Y$. The $\pi/2$ pulses enact the random change of rotation axis, while the $\pi$ is the pulse under test, which may be substituted for any composite pulse for the purpose of comparison. A given randomised benchmarking sequence consists of $l$ computational gates followed by a final reorienting pulse whose direction is chosen such that the the final qubit state may be measured by a $Z$ projective measurement.

It is desirable to understand the behaviour of composite pulses in the presence of weak noise, where resolving measurements of fidelity very close to 100% becomes difficult. Using the technique of randomised benchmarking to amplify the error, it can be seen in Figure 5.8(d) that even in the limit
of weak noise, the WAMF composite pulse consistently outperforms the primitive.

5.6 Conclusion

The focus of this chapter has been on validating the filter function framework for the task of predicting quantum dynamics in realistic environments and demonstrating the relevant physics through construction of error-suppressing composite pulses. The Walsh-modulated pulses presented here complement and systematise the existing formulations. The determination of a restricted search space for error-suppressing pulses in terms of Walsh basis functions provides an efficient method of tailoring composite pulse sequences optimised for known noise environments. The chapter therefore provides both a validation of the general approach, namely the filter function approach to qubit evolution, and a new technique for the specific goal of synthesising error-resistant composite pulses in the presence of time-varying, stochastic qubit noise. Furthermore, the demonstration that filter and Magnus order are distinct has an important consequence for quantum information and control experiments. This consequence is that historic insights into how to tailor control protocol on the basis of knowledge from the field of NMR is insufficient, and a more complete dynamical picture is required, to which the filter function formalism is well suited.
Figure 5.8: (a)-(c) Experimental measurement of single-gate infidelity (left axis) for rotations constructed from various Walsh coefficients in the presence of engineered noise (white dephasing with $\omega_c/2\pi = 20$ Hz). Black dots and line represented calculated fidelity by Schrödinger equation integration (raw and smoothed respectively). All values of $X_3$ for a given $X_0$ implement the same net rotation, indicated by control experiment with no noise. Total rotation time is scaled with $X_3$ to preserve a maximum Rabi rate. Black dashed line (right axis) corresponds to the cost function $A_z$. (d) Randomized benchmarking results (50 randomisations) demonstrating superior performance of modulated gate in the small-error limit (infidelity $< 0.5\%$ per gate). The dots represent each randomisation, the open circles represents the mean bright state probability, and the solid lines are smoothed fits.
Chapter 6

Characterising Frequency Standard Instabilities

6.1 Introduction to frequency standard stabilisation

The problem of stabilisation of a frequency standard may be considered to have the same basic structure as the problem of qubit control. In frequency standards, the noisy dynamics of a classical device such as a laser is controlled by locking to some characteristic frequency of a quantum system, e.g. the qubit splitting frequency. Frequency stability is a chief criterion for evaluating a frequency standard [19], and the vast majority of research in the field focus on breaking stability records by hardware improvements, recently reaching frequency deviations at the $10^{-18}$ level [8, 34]. This chapter presents a platform-independent, software technique for improving the stability of frequency standards, in which statistical correlations between measurements are used to predict the time-domain noise trajectories of frequency. An important insight of this part of the thesis is that the standard operating protocols of frequency standards, such as Ramsey interrogation and feedback correction, may be comprehended using the same descriptive framework as that of the measurement of the stability of frequency standards, such as variance metrics and transfer functions. The stability improvements shown in this chapter, which are informed by real-world experimental parameters, are compatible with a wide range of existing frequency standard technologies.

The vast majority of cutting-edge frequency standards are classified as passive, which means that they consist of a local oscillator (LO) that produces a signal e.g. as a laser, and a passive reference to which the frequency of the signal is locked e.g. an atomic transition. Traditional techniques of locking involve a simple feedback loop, in which a measurement of the frequency deviation of the signal is used to immediately correct the LO frequency, producing a more stable ‘locked local oscillator’ (LLO) signal. Such LO frequency deviations, quantified in terms of variance metrics, may be naturally expressed in the same filter transfer function language as the qubit noise problem. The transfer function approach may be used to calculate the time-correlations between multiple measurement outcomes, allowing for future trajectories of the LO frequency noise to be predicted. Transfer-function-based prediction may be used to improve the accuracy of the feedback lock, leading to a novel method of frequency control known as predictive hybrid feedforward.

This chapter and the next chapter present work that is available as a pre-print [68] which is reproduced in Appendix C. This chapter is organised as follows. Section 6.2 provides the mathematical background to the method of sampling frequency noise in the time domain and expressing the variance of those measurement samples. Section 6.3 derives a novel transfer function form that captures the covariance between two measurements, allowing for the extension of the transfer function forms to include locked local oscillator variance quantities, which are presented for the first time in Section 6.4.
6.2 Filter function approach to frequency standards

The type of noise of interest to the frequency standard community is frequency noise of the local oscillator (LO), which for this purpose is assumed to dominate the noise of the qubit, which acts as a ‘clean’ frequency reference for the LO. The type of metric used to quantify the effect of noise on the LO frequency stability is variance, which is found by successive measurement of the frequency fluctuations. In contrast to the unitary qubit dynamics described in the previous section, the frequency standard is a closed loop control system. There are several variance metrics used by the community that are naturally expressed in the same filter transfer function language as the universal qubit noise problem.

6.2.1 Time-average sampling

The standard method of measuring frequency deviations between an LO and a qubit reference is Ramsey interrogation [65] (originally referred to as the ‘method of separated fields’), which involves performing two \( \frac{\pi}{2} \) rotations of the Bloch vector separated by a long interrogation period of duration \( T^{(R)} \). The frequency fluctuations during the interrogation period result in an axis shift of \( \phi \) between the two \( \frac{\pi}{2} \) rotations, and hence a difference in the final state \( Z \)-projection of

\[
\Delta P_\uparrow \propto \sin^2 (\phi)
\]

which may be directly measured.

Ramsey interrogation provides the template for a more abstract ‘time average sample’ that may be applied to a broader range of physical systems than the molecular beams and trapped ions to which Ramsey interrogation is native. In this model, an LO frequency noise trace \( y(t) \) is sampled in over discrete time bins labelled \( k: [t^*_k, t^*_k] \), where a modulating sensitivity function \( g(t) \in [0, 1] \) captures the contribution of \( y(t) \) to the final measured average over the whole interval of \( \bar{y}_k \). The definition of the \( k \)th sample is thus

\[
\bar{y}_k = \frac{1}{T^{(R)}_k} \int_{t^*_k}^{t^*_k} y(t) g(t - t^*_k) dt
\]

where the \( k \)th Ramsey time is \( T^{(R)}_k \equiv t^*_k - t^*_k \). All variance metrics for LO instability are calculated from sequences of such samples.

For ideal Ramsey interrogation with infinitely fast \( \pi/2 \) pulses, \( g(t) \) has a simple rectangular functional form

\[
g(t) = \begin{cases} 1 & \text{for } 0 < t < T^{(R)}_k \\ 0 & \text{otherwise} \end{cases}
\]

in which case \( \bar{y}_k \) reduces to a simple time-average over \( [t^*_k, t^*_k] \).

For non-ideal cases where the \( \pi \) time \( \tau_\pi > 0 \), the sensitivity function is given by [67]

\[
g(t) = \begin{cases} \frac{\sin (t\pi/2\tau_\pi)}{\pi/2\tau_\pi} & \text{for } 0 < t < \tau_\pi \\ 1 & \text{for } \tau_\pi < t < T^{(R)}_k - \tau_\pi \\ 1 - \sin \left( (t - T^{(R)}_k + \tau_\pi)\pi/2\tau_\pi \right) & \text{for } T^{(R)}_k - \tau_\pi < t < T^{(R)}_k \\ 0 & \text{otherwise} \end{cases}
\]

More complicated sensitivity functions, such as the Hadamard window [66] and triangular windows [15], may be used to find probe specific parts of the noise spectrum.

In these experiments \( \tau_\pi \ll T^{(R)}_k \), so the rectangular sensitivity function (6.3) is used exclusively.

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6.2.2 Variances in the frequency domain

It is useful to derive expressions for different variance metrics in terms of the known frequency noise PSD and the sensitivity functions of the interrogation scheme used. In a similar way to the derivation of the frequency-domain fidelity expression for universal qubit noise, the Wiener-Khinchin theorem can be used to derive filter transfer functions that capture the spectral effect of particular interrogation schemes. Some of these variance metrics pertain to a particular measurement in the sequence and are found by deviations over the ensemble, e.g. true and Allan variances, while others are found by calculating the deviations among a sequence of measurements belonging to a single run, e.g. sample variance [68].

An ideal variance metric that cannot be realised experimentally is the frequency variance, which is the variance over the ensemble \( E \) of \( y(t) \), corresponding to an instantaneous sample at time \( t \). The frequency variance is written \( \text{Var}[y(t)] \):

\[
\text{Var}[y(t)] = E[y(t)^2] - E[y(t)]^2
\]

(6.5)

\[
= E[y(t)^2]
\]

(6.6)

due to the zero-mean assumption \( E[y(t)] = 0 \).

The simplest experimentally-useful variance metric is called the true variance \( \sigma^2_y(k) \) [66], defined

\[
\sigma^2_y(k) = E[\bar{y}_k^2]
\]

(6.7)

\[
= E\left[\frac{1}{T_k^{(R)}} \int_{t_k^s}^{t_k^e} y(t - t_k^s)^2 \, dt\right]
\]

(6.8)

where the zero-mean assumption on \( y(t) \) results in \( E[\bar{y}_k^2] = 0 \). Defining a normalised, time-reversed sensitivity function on the assumption that \( g(t) \) is time-reversal symmetric about \( t_m^k \), the centre point of \([t_k^s, t_k^e]\)

\[
\bar{g}(t_m^k) = \frac{g(t - t_k^s)}{T_k^{(R)}}
\]

(6.9)

which allows the expansion of (6.7)

\[
\sigma^2_y(k) = E\left[\left( \int_{t_k^s}^{t_k^e} y(t)\bar{g}(t_m^k - t) \, dt \right)^2\right]
\]

(6.10)

\[
= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} E[y(t)y(t')]\bar{g}(t_m^k - t)\bar{g}(t_m^k - t') \, dt \, dt'
\]

(6.11)

\[
= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} R_{yy}^{TS}(t' - t)\bar{g}(t_m^k - t)\bar{g}(t_m^k - t') \, dt \, dt'
\]

(6.12)

Applying the Wiener-Khinchin result to the PSD and Fourier transforming the sensitivity function, similarly to section 4.3.3, gives

\[
\sigma^2_y(k) = \frac{1}{2\pi} \int_0^{\infty} S_y(\omega) \left| G_k(\omega) \right|^2 \, d\omega
\]

(6.13)

where \( \left| G_k(\omega) \right|^2 \) is the transfer function for the \( k \)th sample. For the case of rectangular \( g(t) \), the
transfer function has the simple form

$$|G_k(\omega)|^2 \equiv \left| \int_{-\infty}^{\infty} \bar{g}(t^n_k - t) e^{i\omega t} dt \right|^2$$

$$= \frac{\sin^2 (\omega T_k^{(R)}/2)}{(\omega T_k^{(R)}/2)^2}$$

(6.14)

(6.15)

Another important metric for frequency instability is the Allan variance $A\sigma_y^2(k)$ [2], which found by a two-piece rectangular function that covers two adjacent equal-duration interrogation bins with zero dead time between them

$$g(t) = \begin{cases} -1 & \text{for } 0 < t < T^{(R)} \\ 1 & \text{for } T^{(R)} < t < 2T^{(R)} \\ 0 & \text{otherwise} \end{cases}$$

(6.16)

where $T_k^{(R)} = T_{k+1}^{(R)}$ for all $k$ by the uniformity requirement of the Allan variance definition. The resulting transfer function is

$$|A\sigma_y G(\omega)|^2 = \frac{2 \sin^4 (\omega T^{(R)}/2)}{(\omega T^{(R)}/2)^2}$$

(6.17)

and hence the Allan variance is given by the overlap integral

$$A\sigma_y^2(k) = \frac{1}{2\pi} \int_0^{\infty} S_y(\omega) |A\sigma_y G(\omega)|^2 d\omega$$

(6.18)

This thesis relies on measures of frequency stability such as the true variance and sample variance, rather than the more commonly employed Allan variance. This selection has been deliberate as the form of the Allan variance specifically masks the effect of LO noise components with long correlation times. In fact the Allan variance, taking the form $A\sigma_y^2(k) = \frac{1}{2} \text{E}[(\hat{y}_{k+1} - \hat{y}_k)^2]$ is employed by the community in part because it does not diverge at long integration times $\tau$ due to LO drifts, as would the sample or true variance [74, 5, 66, 28]. The Allan variance is most appropriate when comparing the stability, over a range of time scales, of frequency standards where both LO and reference (i.e. qubit) contribute to overall instability [23]. In this system, where LO frequency noise dominates the relatively stable qubit, alternative metrics that assume a fixed reference frequency e.g. true and sample variance more useful.

The third metric of interest is the sample variance, which is defined as the variance of a sequence of samples

$$\sigma_y^2[N] \equiv \frac{1}{N - 1} \sum_{k=1}^{N} (\bar{y}_k - \frac{1}{N} \sum_{l=1}^{N} \bar{y}_l)$$

(6.19)

where the use of brackets for the sample index indicates that the variance is calculated over the first $N$ samples. Since this variance is based on data from only a single run, a more robust measure is the expected value of the sample variance over the ensemble. The expected value of the sample variance can be expressed in terms of the true variance $\sigma^2(k)$ and a novel quantity called the covariance $\sigma(k, l)$:
Figure 6.1: The sum and difference functions for two time-separated samples \( \bar{y}_i \) and \( \bar{y}_j \). These are time-domain functions that capture the sensitivity of a pair of measurements, modulated by the zeroth-order Walsh function (sum sensitivity) and the first-order Walsh function (difference sensitivity). Expressing measured samples in terms of these modulated functions constitutes a basis rotation of 45\(^\circ\), which allows for direct calculation of the correlation and anticorrelation between the two original samples.

Even though expressed as a nested sum over measurement indices \( k, l \), this expression for the expected value of the sample variance is fundamentally a frequency domain quantity, since the true variance and covariance are written in terms of the PSD and relevant transfer functions.

### Covariance in the frequency domain

A vital quantity that has appeared only tangentially in the literature [5] is the covariance between two measurements in a sequence. The covariance is required for calculating transfer function-based expressions for quantities involving time-correlations, e.g. sample variance, and for the predictive protocols introduced in subsequent chapters, which exploit those time correlations.

The covariance \( \sigma(\bar{y}_i, \bar{y}_j) \) of two measurement results indexed \( (i, j) \) is found via a pair of sum and difference sensitivity functions. This formalism compares the variance of sum and difference of the two measurements in order to extract their covariance, using the identity

\[
\sigma^2(A + B) = \sigma^2(A) + \sigma^2(B) - 2\sigma(A, B) \tag{6.21}
\]

We define \( G_{ij}^+(\omega) \) and \( G_{ij}^-(\omega) \) as the Fourier transforms of the sum and difference sensitivity functions \( g_{ij}^+(t) \) and \( g_{ij}^-(t) \). These time-domain functions are plotted in Figure 6.1. The expressions for the sum and difference sensitivity functions for the flat-top case are

\[
g_{ij}^\pm(t) = \begin{cases} 
1, & \text{for } t \in [t_i^s, t_i^e] \\
\pm 1, & \text{for } t \in [t_j^s, t_j^e] \\
0, & \text{otherwise}
\end{cases} \tag{6.22}
\]

from which the sum and difference transfer functions are obtained by Fourier transform:
\[ G_{ij}^\pm (\omega) = \frac{i}{\omega} \left( \frac{e^{-i\omega t_i^e} - e^{-i\omega t_i^s}}{t_i^e - t_i^s} \pm \frac{e^{-i\omega t_j^e} - e^{-i\omega t_j^s}}{t_j^e - t_j^s} \right) \]  

(6.23)

By substituting (6.13) into the identity (6.21) and rearranging terms, it is possible to obtain an expression for the covariance of the two measurements:

\[ \sigma(\bar{y}_i, \bar{y}_j) = \frac{1}{4} \int_0^\infty S_y(\omega) \left( |G_{ij}^+ (\omega)|^2 - |G_{ij}^- (\omega)|^2 \right) d\omega \]  

(6.24)

\[ \equiv \int_0^\infty S_y(\omega) G_{ij}^2 (\omega) d\omega \]  

(6.25)

This covariance expression introduces the concept of the pair covariance transfer function \( G_{ij}^2 (\omega) \), which captures covariance in the frequency domain in an analogous manner to the traditional transfer function \( |G(\omega)|^2 \), which captures variance. This expression is a crucial theoretical result of this thesis. It takes the same overlap integral form as variance quantities of the previous section, capturing instead the covariance between two time-separated measurement windows. Subsequent results on locked local oscillators, as well as the predictive stabilisation of the next chapter, rely on the correlations encapsulated in \( G_{ij} (\omega) \).

In the flat-top case of a sharply rectangular sensitivity function, a closed-form expression for this transfer function can be obtained:

\[ G_{ij}^2 (\omega) = \frac{1}{\omega^2 T_i m T_j m} \left( \cos (\omega (t_j^e - t_i^s)) + \cos (\omega (t_j^s - t_i^e)) - \cos (\omega (t_j^e - t_i^e)) - \cos (\omega (t_j^s - t_i^s)) \right) \]  

(6.26)

This new result permits the calculation of the covariance of any two measurements using (6.25) in a time-domain sequence with arbitrary start and end times for each measurement.

### 6.4 Extending analytic variance expressions to locked local oscillators

The conventional measures for oscillator performance consider only a free-running LO, excluding the effects of feedback locking. In this section explicit analytic forms are presented for variance quantities for locked local oscillators (LLO), i.e. variance in the presence of feedback.

The link between LO and LLO variances is made via a time-domain treatment. Consider the trajectory of the same frequency noise realisation \( y(t) \) in the cases of no correction, \( y^{LO}(t) \) and of correction, \( y^{LLO}(t) \). The relation between these two cases of \( y(t) \) is

\[ y^{LLO}(t) = y^{LO}(t) + \sum_{k=1}^{n} C_k \]  

(6.27)

where \( C_k \) refers to the value of the \( k \)th frequency correction applied to the LLO, \( n \) of which have occurred before time \( t \).

Under traditional feedback, each correction is directly proportional to the immediately preceding measurement outcome: \( C_k = w_k \bar{y}_k^{LLO} \), where \( w_k \) is correction gain. Since \( \bar{y}_k^{LLO} \) is calculated by
convolving \( y^{LLO}(t) \) with a sensitivity function pertaining to the measurement parameters, (6.27) is a recursive equation in general. It is possible to cancel all but one of the recursive terms by setting the correction gain equal to the inverse of the average sensitivity \( \bar{g}_k \equiv \int_0^{T_k} g(t)/T_k \, dt \) of the preceding measurement, i.e. \( w_k = -\bar{g}_k^{-1} \), where the minus sign indicates negative feedback. With this constraint we can write

\[
\tilde{y}_k^{LLO} = \bar{y}_k^{LO} - \frac{\bar{g}_k}{\bar{g}_{k-1}} \, \tilde{y}_{k-1}^{LO}
\]

(6.28)

where \( \bar{g}_k = 1 \) for an ideal Ramsey interrogation and measurement with negligibly short pulses.

The frequency variance of an LLO can be found straightforwardly, by substituting (6.27) into the definition of frequency variance, with the additional substitution of (6.28) for the particular case of traditional feedback:

\[
\text{Var}[y^{LLO}(t)] = E[y^{LLO}(t)^2] - E[y^{LLO}(t)]^2
\]

(6.29)

\[
= E\left[\left(y^{LO}(t) + \sum_{k=1}^{n} C_k\right)^2\right]
\]

(6.30)

\[
= E\left[\left(y^{LO}(t) - \frac{\bar{y}_n^{LO}}{g_n}\right)^2\right]
\]

(6.31)

\[
= E[y^{LO}(t)^2] + \frac{1}{g_n^2} E[(\bar{y}_n^{LO})^2] - \frac{2}{g_n} E[y^{LO}(t)\bar{y}_n^{LO}]
\]

(6.32)

\[
= E[y^{LO}(t)^2] + \frac{\sigma^2_{y^{LO}(n)}}{g_n^2} - \frac{2}{g_n} \sigma(y^{LO}(t), \bar{y}_n^{LO})
\]

(6.33)

where the progression from (6.30) to (6.31) is valid for traditional feedback only, and \( E[y^{LLO}(t)] = 0 \) by assumption and \( n \) indexes the last measurement before \( t \).

The true variance for an LLO can be found in a similar way by substituting (6.28) into the definition of true variance:

\[
\sigma^2_{y^{LLO}(k)} = \text{Var}[\tilde{y}_k^{LLO}]
\]

(6.34)

\[
= \text{Var}\left[\bar{y}_k^{LO} - \frac{\bar{g}_k}{\bar{g}_{k-1}} \, \tilde{y}_{k-1}^{LO}\right]
\]

(6.35)

\[
= \sigma^2_{y^{LO}(k)} + \left(\frac{\bar{g}_k}{\bar{g}_{k-1}}\right)^2 \sigma^2_{y^{LO}(k-1)} - \frac{2}{g_{k-1}} \sigma(\bar{y}_{k-1}^{LO}, \tilde{y}_k^{LO})
\]

(6.36)

where the appropriate forms of the measurement transfer function (6.13) and the pair covariance transfer function can be substituted in to express \( \sigma^2_{y^{LLO}(k)} \) in terms of \( S_y(\omega) \).

The expected value of the LLO sample variance can be found by substituting (6.27) into the definition of the sample variance:
\[
E[\sigma_{yLLO}^2(N)] = \frac{1}{N-1} \sum_{k'=1}^{N} \left\{ \sigma_{yLLO}^2(k') + \frac{1}{N^2} \sum_{p'=1}^{N} \sum_{q'=1}^{N} \sigma(\tilde{y}_{p'}^{LLO}, \tilde{y}_{q'}^{LLO}) - \frac{2}{N} \sum_{l'=1}^{N} \sigma(\tilde{y}_{l'}^{LLO}, \tilde{y}_{l'}^{LLO}) \right\} 
\]

(6.37)

\[
= \frac{1}{N-1} \sum_{k'=1}^{N} \left\{ \left( \sigma_{yLLO}^2(k') + g_k^2 \sum_{r=1}^{[k'/n]} \sum_{s=1}^{[k'/n]} \sigma(C_r, C_s) - 2g_k \sum_{u=1}^{[k'/n]} \sigma(\tilde{y}_k^{LLO}, C_u) \right) + \frac{1}{N^2} \sum_{p'=1}^{N} \sum_{q'=1}^{N} \left( \sigma(\tilde{y}_{p'}^{LLO}, \tilde{y}_{q'}^{LLO}) + g_{p'}g_{q'} \sum_{r=1}^{[p'/n]} \sum_{s=1}^{[q'/n]} \sigma(C_r, C_s) \right) - \frac{2}{N} \sum_{l'=1}^{N} \left( \sigma(\tilde{y}_{l'}^{LLO}, \tilde{y}_{l'}^{LLO}) + g_{l'}^2 \sum_{k=1}^{[l'/n]} \sum_{l=1}^{[l'/n]} \sigma(C_k, C_l) \right) \right\} 
\]

(6.38)

(6.39)

where \(N\) is defined as the total number of measurements and \(n\) as the number of measurements per cycle. The summation signs with unprimed indices are sums over whole cycles (of which there are \([N/n]\)) and the primed indices are sums over all \(N\) measurements. In general, \(E[\sigma_{yLLO}^2(N)]\) contains recursive terms that cannot be concisely expressed in terms of the LO PSD \(S_y(\omega)\) and covariance transfer function \(G^2(\omega)\).

This expression is valid both for the case of traditional feedback where each correction cycle contains only a single measurement (see Figure 7.1b) or novel forms of correction where correction cycles may be interleaved with multiple measurements (see Figure 7.1c).

In the case of traditional feedback, the distinction between primed and unprimed indices disappears and the expression reduces to:

\[
E[\sigma_{yLLO}^2(N)] = \frac{1}{N-1} \sum_{k=1}^{N} \left\{ \left( \sigma_{yLLO}^2(k) + \tilde{g}_k^2 \sum_{r=1}^{k-1} \sum_{s=1}^{k-1} \sigma(C_r, C_s) - 2\tilde{g}_k \sum_{u=1}^{k-1} \sigma(\tilde{y}_k^{LLO}, C_u) \right) + \frac{1}{N^2} \sum_{p=1}^{N} \sum_{q=1}^{N} \left( \sigma(\tilde{y}_p^{LLO}, \tilde{y}_q^{LLO}) + \tilde{g}_p\tilde{g}_q \sum_{r=1}^{p-1} \sum_{s=1}^{q-1} \sigma(C_r, C_s) \right) - \frac{2}{N} \sum_{l=1}^{N} \left( \sigma(\tilde{y}_l^{LLO}, \tilde{y}_l^{LLO}) + \tilde{g}_l^2 \sum_{k=1}^{l-1} \sum_{l=1}^{l-1} \sigma(C_k, C_l) \right) \right\} 
\]

(6.40)

where each term can be expressed in terms of \(S_y(\omega)\) and \(G^2(\omega)\).

The LLO Allan variance can be found by substituting (6.28) into the definition of the Allan variance (6.18):
\[ A \sigma_{y_{LLO}}^2(k) = \frac{1}{2} E[(\bar{y}_{k+1}^{LLO} - \bar{y}_k^{LLO})^2] \]

\[ = \frac{1}{2} E \left[ \left( \frac{\bar{y}_k^{LO}}{g_k} - \frac{\bar{g}_{k+1}}{\bar{g}_k} \bar{y}_k^{LO} + \frac{\bar{g}_k}{g_{k-1}} \bar{y}_{k-1}^{LO} \right)^2 \right] \]

\[ = \frac{1}{2} \left( \sigma_{y_{LO}}^2(k + 1) + \left( 1 + \frac{\bar{g}_{k+1}}{\bar{g}_k} \right)^2 \sigma_{y_{LO}}^2(k) + \left( \frac{\bar{g}_k}{g_{k-1}} \right)^2 \sigma_{y_{LO}}^2(k - 1) \right) \]

\[ + \frac{2\bar{g}_k}{g_{k-1}} \sigma(\bar{y}_k^{LO}, \bar{y}_{k-1}^{LO}) - 2 \left( 1 + \frac{\bar{g}_{k+1}}{\bar{g}_k} \right) \sigma(\bar{y}_k^{LO}, \bar{y}_{k+1}^{LO}) + 2 \left( \bar{g}_k + \frac{\bar{g}_{k+1}}{\bar{g}_{k-1}} \right) \sigma(\bar{y}_k^{LO}, \bar{y}_{k-1}^{LO}) \]

(6.43)

The next chapter takes a key concept from this chapter, the pair covariance transfer function, and uses it to derive a novel predictive method of correction. By contrast to the traditional feedback locking presented in this chapter, the predictive scheme combines multiple measurements to calculate an optimised predictor of the noise trajectory at a future time.
Chapter 7

Transfer Functions for Predictive Stabilisation of Frequency Standards

7.1 Introduction to predictive protocols

The transfer function approach is powerful because it may also be employed to craft new measurement feedback protocols based on predicted noise trajectories. In particular, the aim is to mitigate the deleterious effect of noise on LO frequency stability by combining information from multiple measurements with statistical information contained in the PSD. The key insight is that the non-Markovianity of dominant noise processes in typical LOs – captured through the low-frequency bias in the PSD – implies the presence of temporal correlations in $y(t)$ that may be exploited to improve feedback stabilisation.

The formal basis of the analytic approach is a frequency-domain measure of correlation between time-separated measurements, using the pair covariance transfer function (Equation 6.26). In summary, a covariance matrix is calculated in the frequency domain via transfer functions to capture the relative correlations between sequential measurement outcomes of an LLO, and this matrix is used to derive a linear predictor of the noise at the moment of correction. This predictor provides a correction with higher accuracy than that derived from a single measurement for experimentally-relevant noise spectra, allowing us to improve the performance of the LLO. Since the predictor is found using information from previous measurements (feedback) and a priori statistical knowledge of the LO noise (feedforward), this scheme is called hybrid feedforward. Effectively, the ability to predict the evolution of $y(t)$ by exploiting correlations captured statistically in $S_y(\omega)$ allows feedback stabilisation with increased accuracy and reduced sensitivity to dead time.

This chapter is organised as follows. Section 7.2 derives the linear predictor in terms of the covariance between measurements, via the transfer function formalism presented in the previous chapter. The relation between the linear predictor and the technique of Kalman filtering is discussed. Section 7.3 presents data from numerical simulations of a frequency standard, which demonstrate the superior stabilisation performance of the predictive scheme by contrast to traditional feedback stabilisation. The source MATLAB code for this numerical simulation appears in Appendix D. Section 7.4 presents the experimental setup that allows the trapped-ion system to be used as an emulator of frequency standards via LO noise engineering, and experimental data verifying the effectiveness of the predictive scheme.

7.2 Deriving the linear predictor

In hybrid feedforward, results from a set of $n$ past measurements are linearly combined with weighting coefficients $c_k$ optimised such that the $k$th correction, $C_k$, provides maximum correlation to $y(t_k^c)$ at the instant of correction $t_k^c$ (Figure 7.1c). Assuming that the LO noise is Gaussian, the linear least
minimum mean squares estimator (LMMSE) is optimal, and the optimal value of the correction is given by $C_k = c_k \cdot \bar{y}_k$. The dot product of a set of correlation coefficients $c_k$ derived from knowledge of $S_y(\omega)$ and a set of $n$ past measured samples, $\bar{y}_k = \{\bar{y}_{k-n+1}, \cdots, \bar{y}_k\}$. An $(n + 1) \times (n + 1)$ covariance matrix is defined where the $(n + 1)$th term represents an ideal zero-duration sample at $t_k^n$. In the second line the covariance matrix is written in block form:

$$
\Sigma_k \equiv \begin{bmatrix}
\sigma(\bar{y}_{k-n+1}, \bar{y}_{k-n+1}) & \cdots & \sigma(\bar{y}_{k-n+1}, y(t_k^n)) \\
\sigma(\bar{y}_{k-n+2}, \bar{y}_{k-n+1}) & \cdots & \sigma(\bar{y}_{k-n+2}, y(t_k^n)) \\
\vdots & \ddots & \vdots \\
\sigma(y(t_k^n), \bar{y}_{k-n+1}) & \cdots & \sigma(y(t_k^n), y(t_k^n))
\end{bmatrix} 
\equiv \begin{bmatrix}
M_k \\
F_k \sigma(y(t_k^n), y(t_k^n))
\end{bmatrix}
$$

(7.1)

(7.2)

where each covariance matrix element $\sigma(\bar{y}_i, \bar{y}_j)$ is calculated as a spectral overlap

$$
\sigma(\bar{y}_i, \bar{y}_j) = \frac{1}{2\pi} \int_0^{\infty} S_y(\omega)G_{ij}^2(\omega) d\omega
$$

(7.3)

This novel overlap integral form for covariance, introduced in the previous chapter, comes directly
from the transfer function approach to the problem of covariance, thus linking the predictive correction concept back to the general filter-transfer function formalism that is central to this thesis.

This pair covariance transfer function captures the physics of combining any two Ramsey interrogations of different durations (hence sampling different regions of the LO noise spectrum). The LMMSE optimality condition is then fulfilled for

\[ c_k = \frac{F_k w_k N}{\sqrt{F_k^T M_k F_k}} \]  

(7.4)

where \(w_k\) is an overall correction gain and \(N = \frac{1}{2\pi} \int_0^\infty S_y(\omega) d\omega\) is a normalisation factor related to the overall noise strength in \(S_y(\omega)\).

### 7.2.1 An alternative formulation: Kalman filtering

The field of optimal estimation yields a technique known as Kalman filter or linear quadratic estimation, which has close affinity with the predictive scheme presented above, and developed independently. Optimal estimation seeks to estimate the evolution of a system given a physical model (in this case, the statistics captured by the PSD) and a series of measurements. Both the physical model and the measurement may contain uncertainty. The Kalman filter aims to optimally reconstruct the system evolution given that information, and may be extended to predict future evolution. The goals of optimal estimation thus overlap with the aim of the transfer-function-based predictive hybrid feedforward technique.

This derivation of the Kalman gain vector, which plays the same role as the weighting vector \(c_k\) above, follows [39]. Working with in the discretised time domain consisting of discrete-time samples, the \(k\)th measurement outcome is represented as an \(m \times 1\) vector \(y_k\) based on an underlying state \(n \times 1\) vector \(x_k\) and an \(p \times 1\) applied control vector \(u_k\) applied to the state, where \(k\) indexes the time-step:

\[ y_k = H_k x_k + v_k \]  

(7.5)

\[ x_k = J_k x_{k-1} + G_k u_k \]  

(7.6)

where \(H_k\) is a \(m \times n\) matrix capturing the measurement transformation, \(J_k\) a \(n \times n\) matrix capturing a model of the dynamical process affecting the state, \(G_k\) a \(n \times p\) matrix capturing the action of noise on the state and \(v_k\) a \(m \times 1\) measurement noise vector. The control vector \(u_k\) in the conventional nomenclature of Kalman filtering refers to applied control, but since in this case the only perturbation to the system frequency is LO noise, the thesis treats \(u_k\) as the noisy term in the equation.

To specify this system to the frequency standard problem examined in this chapter, the following assumptions would be made: \(m = 1\) (single degree of freedom) and \(v_k = 0\) (negligible measurement noise). The derivation is presented here in the more general form without these assumptions.

The estimator for the measured outcome is denoted \(\hat{y}_{k|k-1}\), which may be interpreted as ‘the estimate for \(y_k\) given the set of measured outcomes \(\{y_1, \cdots, y_{k-1}\}\)’, and is defined

\[ \hat{y}_{k|k-1} = H_k \hat{x}_{k|k-1} + \hat{v}_{k|k-1} \]  

(7.7)

where the estimator \(\hat{x}_{k|k-1}\) is a prediction of the actual state \(x_k\) based only on the dynamical model. \(\hat{v}_{k|k-1}\) is interpreted similarly, as an estimate of the effect of measurement noise. The residual between the estimated measurement outcome and the actual measured outcome, called the ‘innovation’ in this context, is given by

57
\[ z_k = y_k - \hat{y}_{k|k-1} \]  
\[ = y_k - H_k \hat{x}_{k|k-1} \]  
(7.8)

since it is assumed that measurement noise is uncorrelated with previous measurements, so \( E[v_k y_k] = 0 \) for all \( l < k \).

From the relation of the state estimate from step to step that follows directly from (7.6)

\[ \dot{x}_{k|k-1} = J_k \dot{x}_{k-1|k-1} + G_k u_k \]  
(7.10)

and from the definition of the covariance matrix of the state residual \( P_{k|k} \equiv \text{Cov}[x_k - \hat{x}_{k|k}] \), it is found

\[ P_{k|k-1} = J_k P_{k-1|k-1} J_k^T \]  
(7.11)

It is important to note that the term ‘covariance matrix’ pertaining to \( P_k \) does not explicitly capture covariance over multiple values of \( k \), as does the covariance matrix \( \Sigma_k \) over the \( n \) previous measurements, in the predictive hybrid feedforward calculation of the previous section. Rather, the covariance matrix in the Kalman filter derivation \( P_k \) captures correlations across the elements of \( x_k \), i.e. the multiple dimensions of the state space. The time-correlations appear in the Kalman filter in its nature as a recursive filter, such that the dependence of \( P_{k|k} \) on \( P_{k|k-1} \) reflects the cumulative effect of correlations between measurements. To emphasise this distinction between the explicit correlations across the state space captured by the covariance matrix and the implicit time-correlations captured in the recursive filter, the notation \( \sigma(x_k, x_l) \) is used to refer to covariance between points in time labelled \( k, l \), while \( \text{Cov}[x] \) is used to refer to covariance between the elements of vector \( x \).

The covariance of the innovation is defined \( S_k \equiv \text{Cov}[e_k] \), and so may be expanded to

\[ S_k = H_k P_{k|k-1} H_k^T + R_k \]  
(7.12)

where \( R_k = \text{Cov}[v] \).

The crux of the Kalman filtering approach is that the update to the state estimate \( \ddot{x}_{k|k} \), i.e. the optimal estimate given the latest information, is expressed as a linear combination of the innovation \( z_k \) and the Kalman gain \( K_k \)

\[ \ddot{x}_{k|k} = \dot{x}_{k|k-1} + K_k z_k \]  
(7.13)

where the Kalman gain is defined

\[ K_k = P_{k|k-1} H_k^T S_k^{-1} \]  
(7.14)

where given certain optimality conditions, the Kalman gain minimises the innovation, i.e. the error between the estimated and measured value for \( y_k \).

The predictive hybrid scheme may be understood as a specialised Kalman filter, where \( y_k \) is \( 1 \times 1 \), and the vector \( x_k \) represents a string of previous measurements. Hence the elements of the state-space vector \( x_k \) are chosen to be a ‘recent history’ of the system. This modification allows the Kalman filter to capture time-correlations more explicitly than in the usual formulation, since the state space explicitly includes past measurements.

The Kalman filter and the predictive hybrid scheme are compatible. The frequency-domain approach of the predictive hybrid scheme is preferred because of its accessibility to experimental characterisation (e.g. the PSD) and its mathematical consistency with the transfer functions already known
in the frequency standard community. This formal correspondence allows for the combination of insights from several different research communities: frequency standards, optimal control and quantum control, to produce new results. Kalman filtering has already been applied to an ensemble of frequency standards, *viz.* the weighted combination of multiple clock signals into a more stable composite signal [27]. The single-clock application of the technique may work well in conjunction with multiple-clock time standard schemes.

7.3 Numerical simulation of frequency standard protocols

In the practical setting of a frequency standard experiment, it is necessary to improve both the accuracy of each correction, by maximising the correlation between $C_k$ and $y(t_c^k)$, and the long-term stability of the LLO output, captured by the variance metrics. In order to test the general performance of hybrid feedforward in different regimes, numerical simulations are performed of noisy LOs with user-defined statistical properties, characterised by $S_y(\omega)$. An ensemble $E$ of realisations of $y(t)$ is pseudorandomly generated with statistics given by $S_y(\omega)$. The simulations are performed using a suite of custom-designed MATLAB scripts. The simulated ‘noisy traces’, representing trajectories of $y(t)$ in an ensemble of realisations, are used to calculate measures such as the sample variance over a sequence of simulated measurement samples with user-defined Ramsey measurement times and dead times. In these calculations it may assumed that the LO is either free running, experiencing standard feedback, or employing hybrid feedforward. The calculations include various noise power spectra, with tunable high-frequency cutoffs, including ‘flicker frequency’ ($S_y(\omega) \propto 1/\omega$), and ‘random walk frequency’ ($S_y(\omega) \propto 1/\omega^2$) noise, as appropriate for experiments incorporating realistic LOs.

7.3.1 Correction accuracy

The first performance criterion is the correction accuracy associated with a single correction cycle, defined as the extent to which a correction brings $y_{LLO}(t) \to 0$ at the instant of correction, $t = t_c^k$. The metric for correction accuracy is defined as the inverse of frequency variance at $t_c^k$ relative to the free-running LO

$$A_k \equiv \frac{E[y_{LO}^2(t_c^k)]}{E[y_{LLO}^2(t_c^k)]} \quad (7.15)$$

Closed form analytic expressions for correction accuracy may be calculated in terms of elements of the covariance matrix. A consideration of a single cycle can provide a value for the frequency variance $E[y_{LLO}^2(t_c^k)]$ in terms of covariance matrix elements, which in turn provides a metric for the correction accuracy of hybrid feedforward:

$$A_k \equiv \frac{\langle y_{LO}^2(t_c^k) \rangle}{\langle y_{LLO}^2(t_c^k) \rangle} \quad (7.16)$$

$$= \left( 1 + w_k^2 - w_k \frac{|F_k|^2}{\sqrt{F_k^T M_k F_k}} \right)^{-1} \quad (7.17)$$

Tunability in the hybrid feedforward protocol comes from the number of measurements to be combined, $n$, in determining $\{C_k\}$ as well as the selected Ramsey periods, permitting an operator to sample different parts of $S_y(\omega)$. As an example, the predictor is fixed to consider $n = 2$ sequential measurements and permit the Ramsey durations to be varied as optimization parameters. A Nelder-Mead simplex optimization over the measurement durations finds that a hybrid feedforward protocol consisting of a long measurement period followed by a short period maximises correction accuracy (Figure 7.2a). This structure ensures that low-frequency components of $S_y(\omega)$ are sampled but the
measurement sampling the highest frequency noise contributions are maximally correlated with \( y(t_k) \). With \( S_y(\omega) \propto \frac{1}{\omega} \) and \( S_y(\omega) \propto \frac{1}{\omega^2} \), correction accuracy is improved under hybrid feedback while the rapid fluctuations in \( y(t) \) arising from a white power spectrum mitigate the benefits of hybrid feedforward, as expected. In the parameter ranges studied numerically, correction accuracy is maximised for \( n = 2 \) to 3, with diminishing performance for larger \( n \).

In all locked frequency standards, repeated measurements and corrections provide long-term stability. Instability is a measure of how the output frequency of the LLO deviates from its mean value.

### 7.3.2 Long-term stability

In all locked frequency standards, repeated measurements and corrections provide long-term stability. Instability is a measure of how the output frequency of the LLO deviates from its mean value.

![Figure 7.2](image-url)  

**Figure 7.2**: (a) Calculated correction accuracy of the first correction for hybrid feedforward normalised to feedback \((A^{(FB)} = 1)\), under different forms of \( S_y(\omega) \) as a function of the ratio of Ramsey periods between the two measurements employed in constructing \( C_k(2) \). Correction accuracy for feedback is calculated assuming the minimum Ramsey time; thus for the ratio of Ramsey measurements taking value unity on \( S_y(\omega) \) the \( X \) axis, the hybrid feedforward scheme takes twice as long as feedback. Inset: depiction of the non-interleaved option for hybrid feedback correction. (b) Calculated sample variance for interleaved hybrid feedforward, as a function of measurement number \( N \). The duty cycle of the measurements is fixed at 10\%. Data presented as the normalised ratio of \( E[\sigma_y^2[N]]^{(FB)}/E[\sigma_y^2[N]]^{(HFF)} \) in order to demonstrate improvement due to hybrid feedforward (larger numbers indicate smaller sample variance under hybrid feedforward). Calculations assume \( S_y(\omega) \propto \frac{1}{\omega} \), with a high-frequency cutoff \( \omega_c/2\pi = 100/T_c \) and \( S_y(\omega) \propto \frac{1}{\omega^{1/2}} \) with a cutoff frequency \( \omega_c/2\pi = 1/T_c \), demonstrating the importance of high-f noise near \( \omega/2\pi = T_c^{-1} \). PSDs with different \( \omega \) dependences are normalised to have the same value at \( \omega_{low} = 1/100T_c \). (c) Calculated \( E[\sigma_y^2[N]] \) for \( N = 20 \) as a function of duty cycle, normalised to the sample variance for the free-running LO. Data above red dashed line indicate that the standard feedback approach produces instability larger than that for the free-running oscillator. Both data sets assume \( S_y(\omega) \propto \frac{1}{\omega} \), with \( \omega_c/2\pi = 100/T_c \). Crosses represent data with ten noise spurs superimposed on \( S_y(\omega) \), starting at \( \omega/2\pi = 1.15T_c^{-1} \), and increasing linearly with step size 0.15\( T_c^{-1} \).
over time, and the chosen metric for instability is the sample variance of a time-sequence of measurement outcomes averaged over an ensemble of noise realizations, $\text{E}[\sigma^2_y[N]]$. The interleaved style of hybrid feedforward provides improved long-term stability, as the correction $C_k$ will depend on the set of measurement outcomes $\bar{y}_k = \{\bar{y}_{k-n+1}, \cdots, \bar{y}_k\}$, among which previous corrections have been interleaved, as illustrated in Figure 7.1c.

Figure 7.2b shows the resulting normalised improvement in $\text{E}[\sigma^2_y[N]]$ up to $N = 100$ measurements, calculated using feedback and hybrid feedforward with $n = 2$, and assuming uniform $T_R$. Clear improvement (reduction) in $\text{E}[\sigma^2_y[N]]$ is observed when using the hybrid feedforward approach, with benefits of order $5 - 25\%$ of $\langle \sigma^2_y[N] \rangle$ relative performance improvement over standard measurement feedback. Data is presented for different functional forms of $S_y(\omega)$, including low-frequency dominated flicker noise ($\propto 1/\omega$), and power spectra ($\propto 1/\omega^{1/2}$) with more significant noise near $T_c^{-1}$. The benefits of our approach are most significant in the long term when high-frequency noise reduces the efficacy of standard feedback.

The improvement provided by hybrid feedforward is most marked for low duty cycle $d$, defined as the ratio of the interrogation time to total cycle time: $d = T^{(R)}/T_c$. As $d \to 1$ the feedback and hybrid feedforward approaches converge, as standard feedback corrections become more effective as dead time is shortest. However as the dead time increases, feedback efficacy diminishes until $\langle \sigma^2_y[N] \rangle$ for the feedback-locked LO approaches that for the free-running LO (value unity in Figure 7.2c). In this limit the utility of the measurement-feedback diminishes as the LO noise evolves substantially during the dead time, but even here knowledge of correlations in the noise allows hybrid feedforward to provide significant gains in stability. The benefit afforded by hybrid feedforward is reduced in cases of high duty cycle because the loss of information due to dead time, which is what hybrid feedforward specifically targets, contributes proportionally less to the overall error. Other sources of error such as measurement noise begin to dominate the instability in high duty cycle cases, thereby setting a limit of the effectiveness of hybrid feedforward. Figure 7.2c illustrates that in the presence of a typical $1/\omega$ power spectrum, the presence of noise spurs near $\omega/2\pi = T_c^{-1}$ results in certain regimes where standard feedback makes long-term stability worse, while feedforward provides useful stabilization. Exact performance depends sensitively on the form and magnitude of $S_y(\omega)$, but results demonstrate that systems with high-frequency noise content around $\omega/2\pi \approx T_c^{-1}$ benefit significantly from hybrid feedforward.

### 7.4 Experimental emulator for frequency standards

#### 7.4.1 Frequency measurement technique

The development of noise engineering in this system allows it to be used as an emulator for a wide variety of frequency standard systems. The engineered noise PSDF may be tailored to match those reported in real experimental systems, e.g. optical lattice clocks [34, 8], trapped single-ion clocks [16], atomic fountain clocks [73], crystal sapphire oscillators [31, 57], among other technologies. The timing of the Ramsey interrogation intervals may be set arbitrarily to mimic the real duty cycle limitations experienced by such systems. The trapped Yb+ microwave frequency standard described in this thesis may therefore be used to test software protocols, including the predictive hybrid feedforward scheme described above, in the presence of noise environments that are engineered to emulate any realistic frequency standard system.

The ideal method for sampling a noisy LO frequency $y(t)$ involves a single Ramsey interrogation with $\tau_\pi = 0$ resulting in a perfectly rectangular sensitivity profile $g(t)$. These experiments work in the regime where $\tau_\pi = 50 \mu s$ while $T^{(R)} \geq 100 \text{ ms}$, so the rectangular profile approximation is valid. However, in the context of an experimental frequency standard, performing a Ramsey interrogation in the close vicinity of resonance results in a symmetrical brightness fringe $P_{|\uparrow\rangle}(\omega)$, so that only the magnitude and not the sign of $\bar{y}_k$ can be determined from a single Ramsey interrogation.
Figure 7.3: Spectral diagram of the double Ramsey measurement technique. The LO frequency (solid black line) fluctuates relative to the stable resonance frequency of the qubit (dashed line), with the fractional difference between them defined as $\bar{y}_k$. Due to the symmetry of the brightness peak, the same detuning on either side of qubit resonance gives the same brightness, so a single-Ramsey measurement is ambiguous with respect to the sign of $\bar{y}_k$. By taking two measurements detuned $\Gamma/2$ above and below the nominal LO frequency (black dots), both sign and magnitude of $\bar{y}_k$ may be determined as a function of $\bar{y}_k^+ - \bar{y}_k^-$. 

In order to determine the sign of $\bar{y}_k$, which is required to lock to the centre frequency of the fringe, the Ramsey interrogation is performed twice: once with the microwave carrier detuned $\Gamma/2$ above the fringe centre and a second time detuned by $\Gamma/2$ below the centre, where $\Gamma$ is the full width at half-maximum of the fringe. The sign and magnitude of $\bar{y}_k$ is determined by difference between the measured outcomes $\bar{y}_k^+$ and $\bar{y}_k^-$ obtained from the two interrogation periods. The frequency modulated approach gives sign information and is also more sensitive to $\omega$-fluctuations than interrogating the fringe at the peak [19]. This technique of frequency measurement is depicted in Figure 7.3. In order to perform normalisation to counter photon detector fluctuations, a single normalisation bright state pulse is required, by contrast to the additional dark state normalisation required in the qubit control experiment.

Figure 7.4: Measurements of intrinsic frequency noise in the trapped-ion standard. (a) Time-domain measurements of LO fluctuations relative to the qubit frequency. The Ramsey interrogation period is $T^{(R)} = 100$ ms, with average dead time of $T^{(D)} = 600$ ms between each measurement. (b) Power spectral density calculated from the time-domain data, showing $1/f$ statistics. The source of this characteristic flicker frequency noise signature is believed to be fluctuations in the LO carrier frequency that are produced by instabilities in the Microsemi amplifier, since the bare VSG’s manufacturer-quoted noise spectrum is white. (c) Allan deviation for the LO noise, exhibiting the independence of Ramsey time that is consistent with the $1/f$ noise statistics of the measured PSD in (b).

The frequency standard experiment relies on rectangular-wave FM of the carrier to perform Ramsey spectroscopy of the qubit frequency. This is achieved by using an external arbitrary waveform.
generator (AWG, with model number DG4602 from RIGOL), which produces a rectangular voltage waveform that is sent to the VSG’s external FM port. The frequency and amplitude of the modulating waveform is sent to the generator from the experiment PC, and is triggered by the SpinCore Pulseblaster. Unlike the case of IQM, no discretisation of the FM waveform is necessary.

It is necessary to have an understanding of the intrinsic stability of the trapped-ion system before using it as an emulator with engineered noise. Since frequency stability is the criterion of interest, the frequency deviations between the free-running LO and the qubit are measured over a long period (16384 measurements \(\approx 3\) hours), shown in Figure 7.4. From these time-domain measurements, the power spectral density is calculated and found to fit well to a \(1/f\) flicker frequency noise profile. The calculated Allan variance is independent of the timescale \(\tau\), as expected for flicker noise [66], with best performance at \(A\sigma_y^2(\tau) = 5 \times 10^{-12}\).

\[\text{Figure 7.5} : \text{Schematic diagram of the noise engineering protocol for the frequency standard experiment. The top panel shows the engineered noise trace applied to the LO (red trace), with the user-defined dead times indicated by grey shading to show that the noise trajectory in that period is not measured. The bottom panel shows the control sequence, with microwave pulses in red cross hatch and photon detection windows in grey diagonal hatch.}\]

In order to use the apparatus as an emulator, engineered noise is applied to the LO. For a given user-determined noise PSD, a continuous analytic function representing the time-domain noise trajectory is calculated in \textit{IGOR Pro}. This continuous function is divided piecewise according to user-determined parameters of the measurement protocol: number of measurements, Ramsey interrogation time and dead time. From this piecewise division, engineered \textit{samples} are produced with the appropriate time spacings, and applied to the LO as frequency offsets, imitating the effect of measured frequency noise. The samples are found by integrating the frequency noise trace over the appropriate time interval, but for the sake of computational efficiency, they are calculated by deriving the corresponding phase noise trace and then finding the average gradient across the interval. The benefit of ‘pre-calculating’ the noise trajectory in this way is that the measurement protocol parameters are
highly flexible. Tests of the emulator show that applying engineered noise with a substantially different character to the LO’s intrinsic $1/f$ signature produces measured Allan deviations consistent with the character of the engineered noise. This demonstrates the effectiveness of the emulator, since the engineered noise dominates the intrinsic fluctuations to such an extent that the latter cannot be discerned during noise injection.

![Figure 7.6](image)

Figure 7.6: A demonstration of the engineered noise technique. The red trace is the trajectory of the PC-generated engineered noise trace, which is then imposed on the VSG using the AWG as a source external FM. The black dots are the measured frequency offset of the VSG relative to the qubit frequency, showing that the measured samples match the trajectory of the engineered noise.

In Figure 7.5, the engineered noise trace (solid red) is calculated as a continuous time-domain function that conforms to user-defined PSD parameters. The noise trace is applied directly to the LO in order to mimic the effect of intrinsic LO frequency noise, with the advantage that since the application is software-based, it may be triggered and repeated arbitrarily. This allows the user to freely set the ‘engineered’ dead time $T^{(D)}$, and the noise trace is restarted at the point after a desired dead time period, rather than the actual dead time period enforced by the experimental hardware. The double Ramsey measurement is performed by repeating the noise waveform identically, apart from an FM offset (dashed red lines). This repetition of the waveform ensures that the same engineered noise is being measured both times, once with the LO red-detuned by $\Gamma/2$ and a second time with the LO blue-detuned by $\Gamma/2$, as depicted in Figure 7.3. In combination with the initial bright state normalisation pulse, this control sequence produces an unambiguous measurement of $\tilde{y}_k$ that is robust against photon detection noise. No engineered noise is applied during the normalisation pulse, since its purpose is simply to compensate for intrinsic detection noise. The accuracy of this engineered noise technique is shown in Figure 7.6, where the measured frequency offsets are seen to follow the trajectory of the injected noise.

### 7.5 Experimental verification of stability improvement

An experimental scan of sample variance as a function of the number of samples is shown in Figure 7.7, comparing the stability of the frequency standard emulator under traditional feedback (FB) and the novel predictive hybrid feedforward scheme (HFF). The approximately 10% improvement of HFF over FB in the high $N$ regime (representing long-term stability) is falls within the $5\% – 15\%$ range predicted by the numerical simulation shown in Figure 7.2b. This successful implementation of a predictive HFF correction scheme, and verification of the accuracy of previous simulations, opens the door to an exploration of the scheme in a wide range of realistic noise environments, emulating real-world frequency standards.
Figure 7.7: Experimental demonstration of predictive hybrid feedforward locking. This figure shows measured experimental data for a fixed set of parameters, where the HFF predictor weightings have been optimised to the injected engineered noise spectrum. The engineered noise PSD obeys a $1/\omega$ power law with a high-frequency cutoff $\omega_c = 10$ Hz and a low-frequency cutoff $\omega_b = 1$ mHz with a comb tooth spacing of $\omega_0 = 1$ mHz. The duty cycle of this measurement scheme is $d = 10\%$ with $T_c = 1$s. The optimised weights for the HFF in this scan are [-0.0397, -0.3466, 0.864]. The sample variance as a function of $N$ is lower under hybrid feedforward locking (solid blue) than traditional feedback locking (solid red). The number of samples $N$ is to be understood as the number of samples that contribute to the calculation of sample variance, rather than the number of samples that contribute to the calculation of the hybrid feedforward predictor. Each data point is an average of individual noise realisations (pale red and blue).

It is important to note that even on a single run of the experiment, the predictive hybrid feedforward scheme produces improved correction accuracy, and so improved sample variance over the long term, as indicated by the pale traces in Figure 7.7. Averaging over the ensemble removes the large fluctuations in the low $N$ (short term) regime, showing the superior performance of predictive hybrid feedforward on all timescales (solid lines).

7.6 Conclusion

This thesis seeks to make two primary contributions to the study of frequency standards. First, an extension of the conventional transfer function approach to frequency standards to the novel purposes of (a) characterising locked local oscillators (presented in the previous chapter), and (b) prediction of noise trajectories by exploiting correlations, leading to the novel predictive hybrid feedforward technique. Second, a demonstration of both a numerical simulator and an experimental emulator of frequency standards. Using these tools, the efficacy of the hybrid feedforward scheme is tested in a range of realistic noise settings. The results of these tests suggest that the technique may be of particular use in real frequency standards that are limited by long dead times, such as cutting-edge optical lattice clocks [8].
Chapter 8

Conclusion

8.1 Summary of the thesis

This thesis presents significant theoretical and experimental contributions to the field of precision quantum control. The thesis begins with a unifying abstract treatment of two control problems that share an underlying commonality, those of qubit control and of frequency standards, and proceeds to demonstrate new analysis and improved techniques that are specific to each problem. Chapter 1 introduces the field of precision quantum control and describes, in general terms, the physical system that is investigated in this thesis. Chapter 2 provides a detailed description of the experimental aspects of the project. Chapter 3 derives a mathematical formalism for characterising noise as a spectral density, which is applied to both control problems. Chapter 4 presents the theoretical underpinnings of the filter function approach to qubit control, via an average Hamiltonian derivation. Chapter 5 presents experimental results showing both verification of the filter function as a characterisation tool and its use in constructing improved error-suppressing composite pulses. Chapter 6 introduces the transfer function approach to the characterisation of frequency standards, presenting novel extensions of the approach to calculate variances for feedback-stabilised local oscillators. A key new concept is developed, the pair covariance transfer function, which captures frequency-domain information pertaining to correlations between time-separated measurements. Chapter 7 presents a novel predictive measurement and correction scheme based on this covariance transfer function, along with numerical simulations and experimental verification of its superior stabilisation performance in comparison to traditional feedback.

8.2 Contributions of the thesis

The fields of quantum control and frequency standards are distinct, though both acknowledge the similarity of their systems and the influence of resonance spectroscopy disciplines, such as NMR and ESR [77, 19]. This thesis seeks to unite the two control problems by showing that they represent different ways of looking at the same physical system: a classical oscillator coherently driving a two-level quantum system (qubit). In the interaction-focussed approach taken here, the experimentalist improves the noise-resistance of the overall system by modifying only the interaction between oscillator and qubit. The thesis demonstrates the unity of the qubit control and frequency standard problems by treating them using the same theoretical formalism, the ‘filter-transfer function formalism’, and performing the experiments on the same apparatus using a novel noise engineering technique that allows the system to emulate either qubit or oscillator noise.

The primary contribution to qubit control presented in Chapter 4 is the application of the filter function approach in semiclassical universal noise environments. This theoretical chapter uses an average Hamiltonian theory to derive novel frequency-domain expressions for the qubit trace fidelity (i.e. the accuracy with which an intended operation is achieved in the presence of noise).

Chapter 5 finds that the fidelity predictions accurately match those measured in experiment,
demonstrating for the first time that the filter function formalism is an effective framework in which to cast universal qubit control in the presence of realistic noise. Furthermore, the chapter systematises a range of known error-suppressing composite pulses in terms of Walsh basis modulation. This systematisation contributes to the understanding of the structure and behaviour of such composite pulses, particularly the conceptual distinction between Magnus and filter order. This distinction becomes important in noise environments that fluctuate more rapidly than the quasistatic case for which the pulses were traditionally designed. The generality of the Walsh-modulation prescription allows the development of novel high-filter-order composite pulses, which are experimentally shown to have improved resistance to noise compared to known pulses.

The contributions in Chapter 6 are the novel extensions of the transfer function approach to characterising noise in local oscillators. The extensions to noise characterisation are a set of new analytic forms for the instability of locked local oscillators, where the literature has previously only provided such forms for free-running oscillators. The basis of these novel theoretical results is the derivation of the ‘pair covariance transfer function’, which is frequency-domain function that captures statistical correlations between a pair of measurements.

Chapter 7 presents the derivation and implementation of a novel method of predictive hybrid feedforward to improve the stability of locked local oscillators. The technique allows multiple measurements to be weighted, given a prior characterisation of the oscillator noise statistics, to produce an optimal estimate of the noise trajectory at future times. Since the technique is flexible with respect to noise spectra and measurement parameters (e.g. dead time), it is platform-independent. The numerical simulations and experimental emulations done in this chapter verify the superior performance of the novel predictive technique in parameter regimes of interest. Given its flexibility, predictive feedforward may provide tangible benefits to existing frequency standard technologies, such as the record-breaking optical lattice clocks, since this technique is a modification to the control protocol only. The affinity of this technique with Kalman filtering techniques suggests the possibility of useful synthesis of insights from optimal control theory beyond what has been presented in this thesis.

8.3 Directions for future research

Both sets of experimental results, those in Chapters 5 and 7, represent starting points for further investigation. As noted above, Chapter 5 presents the first experimental validation of the filter function approach as a means of calculating the fidelity of quantum control operations in the presence of noise. Filter-function-based calculations may be used in other noisy systems to predict the performance of error-suppressing composite pulses in a range of different noise environments. Since the power spectral density is a characterisation tool that is familiar to experimentalists, it is expected that the filter function approach will be a convenient method of predicting and assessing the performance of real-world quantum systems.

Similarly, the experimental result of Chapter 7 is the first demonstration of the improved performance of the novel predictive technique, using concepts from optimal estimation for a single frequency standard. This result, in conjunction with the numerical simulations that give a more extensive picture of the regimes where the technique is effective, provides a starting point for further application and exploration of the predictive approach. Further investigation would involve the testing of the predictive technique for a broad range of experimental parameters, including noise spectra with realistic features such as spurs, a wide range of duty cycles to include the different dead time limitations of different systems. The flexibility of the novel technique in combining measurements of different durations could be integrated with the emulator’s double Ramsey technique to provide further improvements in accuracy. A long-term aim of an exhaustive parameter survey of this kind would be the testing of the predictive technique in other advanced frequency standard systems, via this trapped-ion emulator, to demonstrate the benefits of this control technique to the community at large. Further
exploration of the predictive technique beyond frequency standard applications may lead to broader use for the techniques in such fields as quantum state estimation.
Appendix A

*Nature Physics* publication
Experimental noise filtering by quantum control

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Extrinsic interference is routinely faced in systems engineering, and a common solution is to rely on a broad class of filtering techniques to afford stability to intrinsically unstable systems or isolate particular signals from a noisy background. Experimentalists leading the development of a new generation of quantum-enabled technologies similarly encounter time-varying noise in realistic laboratory settings. They face substantial challenges in either suppressing such noise for high-fidelity quantum operations\textsuperscript{1} or controllably exploiting it in quantum-enhanced sensing\textsuperscript{2–3} or system identification tasks\textsuperscript{4–6}, due to a lack of efficient, validated approaches to understanding and predicting quantum dynamics in the presence of realistic time-varying noise. In this work we use the theory of quantum control engineering\textsuperscript{7–8} and experiments with trapped \textsuperscript{171}Yb\textsuperscript{+} ions to study the dynamics of controlled quantum systems. Our results provide the first experimental validation of generalized filter-transfer functions casting arbitrary quantum control operations on qubits as noise spectral filters\textsuperscript{9–10}. We demonstrate the utility of these constructs for directly predicting the evolution of a quantum state in a realistic noisy environment as well as for developing novel robust control and sensing protocols. These experiments provide a significant advance in our understanding of the physics underlying controlled quantum dynamics, and unlock new capabilities for the emerging field of quantum systems engineering.

Time-varying noise coupled to quantum systems—typically qubits—generically results in decoherence, or a loss of ‘quantumness’ of the system. Broadly, one may think of the state of the quantum system becoming randomized through uncontrolled (and often uncontrollable) interactions with the environment during both idle periods and active control operations (Fig. 1a). Despite the ubiquity of this phenomenon, it is a challenging problem to predict the average evolution of a qubit state undergoing a specific, but arbitrary operation in the presence of realistic time-dependent noise—how much randomization does one expect and how well can one perform the target operation? These considerations motivate the development of novel engineering-inspired analytic tools enabling a user to accurately predict the behaviour of a controlled quantum system in realistic laboratory environments. Recent work has demonstrated that the average dynamics of a controlled qubit state evolution may be captured using filter-transfer functions (FFs) characterizing the control. The fidelity of an arbitrary operation over duration $\tau$, $\chi_\tau(S)$, is degraded owing to frequency-domain spectral overlap between noise in the environment given by a power spectrum $S(\omega)$, and the filter-transfer functions denoted $F(\omega)$ (Methods).\textsuperscript{11–14}

The FF description of ensemble-average quantum dynamics tremendously simplifies the task of analysing the expected performance of a control protocol in a noisy environment as it permits consideration of control as noise spectral filtering. The FFs themselves may be described using familiar concepts such as frequency passbands, stopbands and filter order, enabling a simple graphical representation of otherwise complex concepts in the dynamics of controlled quantum systems (Fig. 1b). Noise filtering, in practice, is achieved through construction of a control protocol (Fig. 1a) which modifies the controllability of the quantum system by the noisy environment over a defined frequency band. Adjusting $F(\omega)$ and changing its overlap with the noise spectrum thus allows a user to change the average dynamics of the system in a predictable way.

To see the importance of this capability we may consider the various tasks that might be of interest in experimental quantum engineering and the role of noise spectral filtering in these applications. In quantum information an experimentalist may aim to suppress broadband low-frequency noise to maximize the fidelity of a bounded-strength quantum logic operation (Fig. 1b, upper trace), and then calculate the residual error. Alternatively, in quantum-enabled sensing or system identification he or she may perform narrowband spectral characterization of a given operation (Fig. 1b, lower trace), where any change in the measured fidelity under filter application represents the signal of interest\textsuperscript{12–16}.

The intuitive nature of this framework is belied by the challenge of calculating FFs for arbitrary control protocols, generally involving time-domain modulation of control parameters such as the frequency and amplitude of a driving field. The nature of quantum dynamics means that the implemented control framework is generally nonlinear; for instance, one finds complex dynamics in circumstances where the noise and control operations do not commute, such as a driven operation ($\propto \sigma_z$) in the presence of dephasing noise ($\propto \sigma_z$). Recent theoretical effort has allowed calculation of FFs for arbitrary single-qubit control and arbitrary universal classical noise\textsuperscript{16,19}, expanding significantly beyond previous demonstrations restricted to the identity operator in pure-dephasing environments\textsuperscript{35}. It

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is this more general case where the impact of noise filtering and the FFs may have the most significant impact on the quantum engineering community, and where experimental tests are vital.

In our experimental system, based on the 12.6 GHz qubit in $^{171}\text{Yb}^{+}$ (Supplementary Methods), we are able to perform quantitative tests of operational fidelity for arbitrary control operations; these may then be compared against calculations of $F_{\chi}(\tau)$ as a fundamental test of FF validity. A key tool in our studies is bath engineering, in which we add noise with user-defined spectral characteristics to the control system, producing well-controlled unitary dephasing or depolarization.

As a first example (Fig. 1c), experimental measurements of operational fidelity for a $\pi$-pulse driving qubit population from the dark state to the bright state, $|0\rangle \rightarrow |1\rangle$, in the presence of engineered time-dependent dephasing noise give good agreement with analytic calculations of $F_{\chi}(\tau)$ using the noise power spectrum and analytic FFs (ref. 10) with no free parameters (Methods). This approach therefore immediately demonstrates the predictive power of the FF formalism.

The FFs for much more complex control, such as compensating composite pulses$^{11,12}$, can be calculated and experimentally validated as well (Fig. 1e). These protocols are commonly used in nuclear magnetic resonance and electron spin resonance in attempting to suppress static offsets in control parameters such as the frequency of the drive inducing spin rotations. Calculating the FFs for these protocols now reveals their sensitivity to time-dependent noise—an important characteristic for deployment in realistic quantum information settings$^{10}$. We experimentally demonstrate a form of quantum system identification (Methods), effectively reconstructing the amplitude-noise filter functions, $F_{\chi}(\omega)$, for two well-known compensating pulse sequences known by the shorthand designations SK1 and BB1 (Supplementary Methods). Again, calculations of $F_{\chi}(\tau)$ match data well over the entire band in the weak-noise limit (Fig. 1f) with no free parameters.

Our choice of characterizing these compensating pulse sequences highlights an important issue in the prediction of ensemble-average dynamics of controlled quantum systems. Ultimately, the underlying physical principles giving rise to the analytic form of $F(\omega)$ are based on the well-tested average Hamiltonian theory$^{20}$ exploited in crafting these pulses. Despite this shared theoretical foundation, the calculation of spectral filtering properties is quite distinct from calculation of quasi-static error terms in a Magnus expansion, with important consequences for average quantum dynamics in realistic time-varying noise environments$^{20}$.

Accordingly, our tests of the FF formalism reveal that compensating pulses designed to suppress errors to high order in a Magnus-expansion framework need not be efficient noise spectral filters (Supplementary Methods and ref. 19). Despite significant differences in their construction—the BB1 protocol is designed to provide higher-order cancellation of Magnus terms than SK1—both of the selected composite pulses provide similar filtering of time-dependent noise, given by the filter order (slope of the FF in Fig. 1e). In the weak-noise limit frequency-domain characteristics...
These simple but powerful validations of the predictive power of the generalized FF formalism now open the possibility of demonstrating the construction of noise filters with a specified spectral response, employing the filter-transfer function as an analytic tool. Filters may take a wide variety of forms as needed by users—including high-pass filters for broadband noise suppression and band-stop filters useful for narrowband noise characterization (Fig. 1b).

In the discussion that follows, we focus on a common setting in which we aim to improve operational fidelity by reducing the influence of broadband non-Markovian noise on a target state transformation. Filters are realized as \( n \) steps of time-domain control operations with tunable pulse amplitude and phase, similar in spirit to compensating composite pulses in NMR (refs 17–19), dynamically corrected gates (DCGs) in quantum information\(^\text{(20,21)}\), and open-loop modulated pulses in quantum control\(^\text{(22,23)}\). However, recalling the difference between Magnus cancellation order and filtering order described above, in this setting we wish to synthesize a filter with arbitrary, user-defined spectral characteristics captured by a cost function, \( A(\Gamma_l) \), to be minimized for a filter represented by \( \Gamma_l(\phi, \tau, \theta) \) (Fig. 2b and Methods).

To provide efficient solutions to filter design we restrict our control space and focus on constructions synthesized using concepts from functional analysis in the basis set of Walsh functions—square-wave analogues of the sines and cosines\(^\text{(24,25)}\) (Fig. 2a). This approach provides significant benefits for our problem\(^\text{(26)}\), but is by no means the only basis set for composite filter construction\(^\text{(27,28)}\).

As an example we synthesize noise filters via weighted linear combinations of Walsh functions, PAL\(_n\)(\( x \)) denoted by the Paley-ordered index, \( k \). These filters are designed to suppress time-varying dephasing noise over a low-frequency stopband while implementing a bounded-strength driven rotation about the \( x \) axis on the Bloch sphere (Supplementary Methods). In this case the Walsh-synthesized waveform dictates an amplitude modulation pattern for the control field over discrete time segments. Importantly, Walsh filter synthesis is compatible with pulse segments possessing arbitrary pulse envelopes, including sequences of, for example, square (used here) or Gaussian pulse segments (Fig. 2b).

Analytic design rules provide simple insights into how one may craft effective modulation protocols, and a Nelder–Mead simplex optimization is used to find high-performing operations as defined by our cost function. Relative to an unfiltered primitive gate, the dephasing filter function, \( F_l(\omega) \), for the simplest four-pulse construction \( W_1 \) shows increased steepness in the stopband (Fig. 2c, red), reducing \( A(\Gamma_l) \) (here the gate performs \( \theta = \pi \)). This measure of filter order may be further increased via construction \( W_2 \), in turn reducing the cost function for optimization (blue shaded area in Fig. 2c). Relating back to earlier demonstrations of filter order in compensating pulses, \( W_2 \) presents an interesting case of a high-order noise filter over the target band which provides only first-order Magnus cancellation.

Filters \( W_1 \) and \( W_2 \) are representative, rather than unique solutions. In Fig. 3b we show the calculated cost function, \( A(\Gamma_l) \), as a function of the Walsh coefficients used in constructing \( W_1 \) and \( W_2 \), giving the modulation profile indicated in Fig. 3a. Blue areas meet our optimized target, indicating useful filters, revealing a wide variety of possible constructions with favourable characteristics. Experimental tests of these protocols reveal that Walsh-modulated waveforms minimizing \( A(\Gamma_l) \) effectively suppress noise in the designated stopband for arbitrary rotation angles (Fig. 3c–e), and outperform standard pulses in the small-error limit germane to quantum information (Fig. 3f). See Methods.

Our focus has been on providing a validated framework for the vital task of predicting quantum dynamics in realistic environments and demonstrating the relevant physics through construction of noise spectral filters. The Walsh-modulated filters

![Figure 2](https://example.com/figure2.png)

**Figure 2** | Synthesis of high-pass amplitude-modulated filters from the Walsh functions. **a.** The first eight Walsh functions used in filter synthesis, \( (P_{10}, P_{20}, P_{30}) \), with maximum-Hamming-weight-indexed functions highlighted in red. **b.** Representative amplitude profiles for filter constructions found via a numerical search over the Walsh basis with four (red, denoted \( W_1 \)) and eight (blue, denoted \( W_2 \)) time steps. Vertical axis represents \( \Omega \), the Rabi rate per time step; negative values indicate \( \pi \)-phase shifts. Synthesis may be performed over square (flat-top) pulse segments or Gaussian-shaped pulse segments, with results differing only in the resulting Walsh coefficients. The matrix representing filter characteristics over eight segments is superimposed on the amplitude profiles for \( n = 4 \), neighbouring segments between red dashed lines are combined. The first row (the angles of rotation in each segment of the filter) is determined via Walsh synthesis, indicated by the vectors \( X^{(n)} \), containing the spectral weights over \( P_{10} \) – \( P_{20} \). In the case of Gaussian pulse envelopes Walsh synthesis sets the first line, \( \phi \). The symbol \( X \) indicates reordering for Hadamard synthesis, with listed coefficients appropriate for square pulse envelopes. **c.** The filter-transfer function for a primitive \( \gamma \) rotation and for synthesized noise filters. Performance improvement over the desired stopband of the filter captured in cost function \( A(\Gamma_l) \), and its difference relative to that for the primitive operation, \( A(\Gamma_l^{(\phi)}) \). Filter \( W_1 \) gives improvement indicated by the red shading, with additional improvement in the cost function given by \( W_2 \) indicated by blue shading.
presented here—based on the achievable frequency-domain filter order—complement existing techniques rather than attempting to provide optimal-performance error-robust gates. Our results on high-pass noise filters, for instance, add to existing compensating pulse sequences designed for quasi-static noise, as well as gate constructions with interleaved dynamical decoupling that seek to periodically ‘refocus’ quantum evolution.\(^{23-32}\)

Importantly, recent work has demonstrated that the filter-transfer function formalism is applicable to multiple-qubit settings where dynamics may be considerably more complex than the single-qubit case.\(^{33-35}\) In addition, ongoing efforts suggest there exists a path towards further extension of the generalized filter-transfer function and noise filtering formalisms to arbitrary control settings involving multiple qubits subject to general noise from non-Markovian classical and/or quantum mechanical environments. We believe that with the validations provided here, this simple extensible framework with precise predictive power will provide a path for experimentalists to characterize and suppress the effects of noise in generic quantum coherent technologies, ultimately enabling a new generation of engineered quantum systems.

**Methods**

The fidelity of a control operation for a single qubit in the presence of a time-dependent environment is reduced as \(S(\tau) = \exp(-t \sqrt{\frac{\gamma}{2}})} \), where \(\chi(\tau) = 1 + \int_0^\infty \sum_{n} \frac{\omega_n S_{\omega_n}(\omega)}{\Gamma_{\omega_n}(\omega)} \tau\) and \(\tau\) is the total duration of the operation. In this expression for fidelity, the integral considers contributions from independent noise processes through their frequency-domain power spectra \(S_{\omega_n}(\omega), \omega_n \in [\omega, 2\omega]\), capturing dephasing along \(\omega\) and amplitude noise co-rotating with a resonant drive field (Supplementary Methods). We employ here the so-called modified filter-transfer function, which subsumes a factor of \(\omega^2\) into the definition of \(F_{\omega}(\omega)\). See refs 6,14 for details.

Experimental measurements involve state initialization in \(|0\rangle\) followed by a control operation—or series of control operations—designed to drive qubit population from the dark state to the bright state, \(|0\rangle\rightarrow |1\rangle\). For instance, tests of filters used for rotations \(\Theta = \pi\) are repeated sequentially such that the net rotation enacted on \(|0\rangle\rightarrow |1\rangle\). (Fig. 3d). The operational fidelity is measured as the probability that the qubit is in the bright state over an ensemble of measurements. Typical experimental uncertainties are limited by measurement fidelity \((\sim 98.5\%)\) and quantum projection noise with maximum value comparable to the measurement infidelity for qubit states near the equatorial plane of the Bloch sphere. In general, a non-Markovian noise bath is engineered with specific properties of interest (see Supplementary Methods for full details). Additional measurement uncertainty of \(\sim 0.5\%\) is added through finite sampling of the infinite ensemble of possible noise realizations. This is visible as fluctuations between neighbouring points in, for example, Fig. 3c–f.

Measurements in Fig. 1c are conducted for a simple \(\pi\) enacted while varying the high-frequency cutoff, \(\omega_0\), of a flat-top engineered non-Markovian dephasing bath (Fig. 1d). As the high-frequency cutoff of the noise is increased and fluctuations fast relative to the control \(\tau_\text{on}\), \(\omega_0\) are added to the noise power spectrum, \(S_\omega(\omega)\), errors accumulate, reducing the measured fidelity. For \(\omega_0/2\pi = 1\) the highest frequency contribution to \(S_\omega(\omega)\) undergoes a complete cycle of oscillation over \(\tau_\text{on}\), indicating that the noise is time-dependent on the scale of a single experiment even for \(\omega_0/2\pi < 1\). We calculate \(F_{\omega}(\omega)\) using the form of the noise and the analytic FF for a driven primitive gate under dephasing,\(^{49}\) finding good agreement with experimental measurements using no free parameters.

Measurements in Fig. 1f employ a narrow-band ‘delta-function’ noise power spectrum swept as an experimental variable, \(\omega_0\). Injected noise takes the form of fixed-frequency amplitude modulation of the near-resonant driving field during application of a control pulse, with strength (modulation depth) parameterized in terms of \(\Omega\), the Rabi rate of the drive. The form of \(F_{\omega}(\omega)\) demonstrates that the calculated fidelity involves an exponentiated value of the FF at frequency \(\omega_0\), meaning that fidelity measurements effectively reconstruct the filter functions. Key features in the data, such as performance-crossover frequencies between primitive and compensating gates and deep notches in the filter at high frequency, are quantitatively reproduced in experimental measurements.

Filter construction presented in Figs 2 and 3 is parameterized as a function of controllable properties of a near-resonant carrier frequency enacting driven operations. An arbitrary \(n\)-segment filter is represented over successive timesteps through the matrix quantity \(\Gamma_{\omega_n}(\theta, \phi, \psi)\) (Fig. 2b); in each segment of duration \(\tau\),
we perform a driven operation generating a rotation through an angle
\[ \theta_l = \int_0^t \Omega_l(t) dt \] about the axis \( \mathbf{n} \) = \( (\cos(\xi(t)),\sin(\xi(t)),0) \), with \( \Omega_l(t) \) the Rabi rate
over the \( l \)th pulse segment.

The value of \( \theta_l \) is chosen to be a power of two, compatible with synthesis over discrete-time Walsh functions. The Walsh functions are piecewise-constant over segments which are integer multiples of base period \( \tau \). This approach brings benefits for the current setting\(^{26}\), for instance, their piecewise-constant construction builds intrinsic compatibility with discrete clocking and classical digital logic, while the well-characterized mathematical properties of the Walsh functions provide a basis for establishing simple analytic filter-design rules, and flexibility in realizing a wide variety of filter forms.

For the filters W1 and W2 presented in the main text, Walsh-synthesis
rules dictate that we implement our filtered rotation by \( \theta_l \) over a
minimum of four discrete steps, permitting synthesis over PAL to
PAIL. Within this small set, the coefficient of PAL, denoted \( X_l \), sets the total rotation angle \( \theta \mod 2\pi \) for the modulated driven evolution, and only non-zero \( X_l \) preserves
symmetry. We experimentally test the performance of four-segment
amplitude-modulated filters by scanning over \( X_l \) for fixed \( X_0 \), denoted by white
dotted lines in Fig. 3b). Values of \( X_l \) mimicking \( A(l) \) (dips in the dashed trace, right axis) also minimize the experimentally measured infidelity in the presence of engineered low-frequency noise (open circles, left axis). This behaviour
is observed for various target rotation angles of interest (Fig. 3c–e), with predicted
shifts in the optimal values of \( X_l \) with changes in \( X_0 \), borne out through
experiment. Filter W2 is constructed over PAL, to PAIL, and has twice as many
timesteps as W1. Interestingly, W1 is a special case of an analytically constructed
dynamically corrected NOT gate (\( \pi \) rotation\(^{27}\)). For details of the Walsh
functions, Walsh synthesis and Walsh-basis analytic design rules see
Supplementary Methods.

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Author contributions
A.S., H.B., D.H. and M.J.B conceived and performed the experiments, built experimental apparatus, contributed to data analysis and wrote the manuscript. T.J.G. conceived the relevant theoretical constructs. J.S., M.C.J. and X.Z. assisted with development of the experimental system and data collection. J.M.J. assisted with data collection.

Additional information
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Experimental noise filtering by quantum control

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Theoretical model

We consider a model quantum system consisting of an ensemble of identically prepared noninteracting qubits immersed in a weakly interacting noise bath and driven by an external control device. Working in the interaction picture with respect to the qubit splitting \(\omega_0\) state transformations are represented as unitary rotations of the Bloch vector. The generalized time-dependent Hamiltonian is then written

\[
H(t) = H_c(t) + H_0(t)
\]

where \(H_c(t)\) describes perfect control of the qubit state, e.g. via an ideal external driving field, and the noise Hamiltonian \(H_0(t)\) captures undesirable interactions with a (universal) noise bath.

The specific forms taken by \(H_c(t)\) and \(H_0(t)\) in this work are given in the sections below, where we treat both dephasing (detuning) and amplitude-damping (coherent relaxation) noise processes. We will begin with this model to craft time-dependent noise filters, and detail this method in the following sections.

Defining the control space

Representing the qubit state on the Bloch sphere, state manipulation maps to a rotation of the Bloch vector in \(\mathbb{R}^3\) and described by the unitary \(U(\theta, \phi) := \exp(-i\frac{\Omega(t)}{2}\sigma_\phi)\), reflecting the homeomorphism between \(SU(2)\) and \(SO(3)\). In effect, the spin operator \(\sigma_\phi := \vec{r} \times \vec{\sigma}\) generates a rotation through an angle \(\theta\) about an axis \(\vec{r}\) defined by the unit vector \(\vec{r} \in \mathbb{R}^3\). For our purpose control takes the form of a composite pulse sequence consisting of \(n\) such unitaries executed over a time period \([0, \tau]\), with the \(l\)th pulse in the sequence written

\[
P_l := U(\theta_l, \phi_l) = \exp \left[ -i \frac{\sigma_\phi}{2} \int_{t_{l-1}}^{t_l} \Omega_l(t) dt \right]
\]

\[
\sigma_{\phi_l} := \cos(\phi_l) \sigma_z + \sin(\phi_l) \sigma_y.
\]

Here \(\Omega_l(t)\) is the Rabi rate with arbitrary amplitude envelope in a single pulse, \(\tau_l = t_l - t_{l-1}\) is the pulse duration, and the spin operator \(\sigma_{\phi_l}\), parametrized by \(\phi_l \in [0, 2\pi]\), generates a rotation \(\theta_l = \int_{t_{l-1}}^{t_l} \Omega_l(t) dt\) of the Bloch vector about an axis \(\vec{r}_l := (\cos(\phi_l), \sin(\phi_l), 0)\) in the \(xy\)-plane.1 This sequence of control unitaries implies a natural partition of the total sequence duration \(\tau\) into \(n\) subintervals \(t_l = [t_{l-1}, t_l], l \in \{1, n\}\), such that the \(l\)th pulse has duration \(\tau_l = t_l - t_{l-1}\) with \(t_{l-1}\) and \(t_l\) the start and end times respectively. Here \(t_0 \equiv 0\) and \(t_n \equiv \tau\).

The control Hamiltonian associated with this composite pulse sequence takes the form

\[
H_c(t) = \sum_{l=1}^{n} G_l(t) \frac{\Omega_l(t)}{2} \sigma_{\phi_l}
\]

where the function \(G_l(t)\) is 1 if \(t \in I_l\) and zero otherwise. The sequence of \(n\) triples \(\{(\theta_l, \tau_l, \phi_l)\}\) completely characterizes the net effect of the applied control \((P_n = P_1(\theta_1, \Omega_1(t), \tau_1, \phi_1))\) at the end of successive pulse applications. We define the \(n \times 3\) composite pulse sequence matrix

\[
\Gamma_n = \begin{bmatrix}
\theta_1 & \tau_1 & \phi_1 \\
\theta_2 & \tau_2 & \phi_2 \\
\vdots & \vdots & \vdots \\
\theta_n & \tau_n & \phi_n
\end{bmatrix}
\]

(5)

to compactly describe any arbitrary \(n\)-pulse control sequence. The entire space of such control forms therefore corresponds to an infinite set of \(\Gamma_n\) matrices ranging continuously over all possible values taken by the control parameters. We denote this set by \(\mathcal{E}_n\) and refer to it as the \(n\)-pulse control space. Written formally

\[
\mathcal{E}_n := \left\{ \Gamma_n | \theta_l, \tau_l > 0, \phi_l \in [0, 2\pi], l \in \{1, ..., n\}, \sum_l \tau_l = \tau \right\}
\]

Noise bath model

We consider semi-classical time-dependent dephasing (detuning) and amplitude damping (relaxation) processes, captured respectively through the appearance of stochastic rotations about \(\sigma_z\) and \(\sigma_\phi := \cos(\phi) \sigma_x + \sin(\phi) \sigma_y\)
\[ H^{(3)}(t) = \beta_3(t) \hat{\sigma}_z \]
strength and vanish under our assumption of zero-mean, Gaussian-distributed random variables. Writing the $O(\xi^0), O(\xi^2), O(\xi^4)$ classes explicitly we have

$$F_{av} = 1 - \langle a_1^2 \rangle - \left[ \langle a_2^2 \rangle + 2\langle a_1 a_2^\dagger \rangle - \frac{\langle a_1 \rangle^2}{3} \right] + \sum_{k=3}^{\infty} O(\xi^{2k})$$

(14)

Immediately we see that there is a collection of terms with equal magnitude arising from different orders of the Magnus expansion (e.g. $a_2^2$ vs $a_1^4$). The individual terms in the series expansion of the fidelity rely on time-domain correlation and cross-correlation functions and convolution with a multidimensional control matrix capturing the effect of the control operations.

The fidelity is thus expressed explicitly in terms of noise correlations and the control matrix. For instance,

$$\langle a_2^2 \rangle = \sum_{i,j=x,y,z} \int_0^t dt_1 \int_0^t dt_2 \langle \beta_i(t_1) \beta_j(t_2) \rangle R_i(t_1) R_j^\dagger(t_2)$$

$$= \sum_{i,j,k=x,y,z} \int_0^t dt_1 \int_0^t dt_2 \langle \beta_i(t_1) \beta_j(t_2) \rangle R_{ik}(t_1) R_{jk}(t_2)$$

(15)

contains all two-point noise cross-correlation functions $\langle \beta_i(t_1) \beta_j(t_2) \rangle$, for $i,j \in \{x,y,z\}$. Higher-order terms contain multipoint correlation functions (this is determined by the sum of subscript indices, as they indicate the expansion-order of the error vector).

We rewrite these terms in the frequency domain, defining the Fourier transform $S_{i_1...i_n}(\omega_1,...,\omega_n)$ of an $n$-point cross-correlation function via

$$\langle \beta_i(t_1) \beta_j(t_2) \rangle \equiv \frac{1}{(2\pi)^n} \int d\omega_1...d\omega_n S_{i_1...i_n}(\omega_1,...,\omega_n) e^{i(\omega_1 t_1 + ... + \omega_n t_n)}$$

(16)

The fidelity above can then be rewritten as

$$F_{av} = 1 - \sum_{n=2}^{\infty} \frac{1}{(2\pi)^n} \sum_{i_1...i_n} \int d\omega_1...d\omega_n S_{i_1...i_n}(\omega_1,...,\omega_n) R_{i_1...i_n}(\omega_1,...,\omega_n)$$

(17)

where $R_{i_1...i_n}(\omega_1,...,\omega_n)$ is determined solely by the control matrix and increases in complexity at higher order. Explicit expressions for terms to arbitrary order are found in [11].

**First-order fidelity approximation**

Here we briefly explain the choice of fidelity metric used in the figures of the main text to produce the theory curves against which our experimental data is compared. Experimental fidelities are determined by measuring the brightness of the ion cloud after completing the control sequence, effectively yielding a projective measurement onto the $|\uparrow\rangle$ state. We denote this metric by $F_I(\tau) \in [\frac{1}{2},1]$ and refer to it as the state fidelity, with lower and upper bounds corresponding to complete decoherence and perfect fidelity respectively.

If the noise is sufficiently weak ($\xi^2 \ll 1$) we may truncate the series expansion for fidelity after the $O(\xi^2)$ term yielding the approximation

$$F_{O(1)} = 1 - \langle a_1^2 \rangle.$$

(18)

Here the term which dominates the measured infidelity is $\langle a_1^2 \rangle := \langle a_1(\tau) a_1^\dagger(\tau) \rangle$, defined as the ensemble averaged modulus square of the first order error vector $a_1(\tau)$. Assuming wide sense stationarity, independence and zero mean of both noise fields $\beta_\alpha(t)$ and $\beta_\beta(t)$ we may derive a spectral representation of $\langle a_1^2 \rangle$ of the form

$$\langle a_1^2 \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega}{\omega^2} S_{a}(\omega) F_a(\omega) + \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega'^2} S_{a}(\omega') F'_a(\omega').$$

(19)

Here $S_a(\omega)$ and $S_a(\omega)$ denote the dephasing and amplitude noise PSDs. The dephasing $F_a(\omega)$ and amplitude $F'_a(\omega)$ filter functions, on the other hand, capture the spectral response of the control sequence and are completely defined as functions of the control sequence.

As the integrated noise content increases, however, higher-order error contributions must be included; neglecting to do leads to the unphysical result that $F_{O(1)} \leq 0$ when $\xi^2 \geq 1$. Although computation of all higher-order contributions is challenging we may gain some insight into the full expansion by considering terms of the form $\langle a_1^{2m} \rangle \equiv \langle a_1^2 \rangle^m$ in each class $O(\xi^{2m})$. This collection of terms is obtained by setting $a_2^2 \rightarrow a_1^2$ in Eq. 10, effectively including only the first-order Magnus expansion.
term in the expansion for Fidelity, yielding
\[
\mathcal{F}_{\mathcal{O}(1)}(\tau) = \frac{1}{2} \left[ 1 + \sum_{m=0}^{\infty} (-1)^m \frac{2^{2m}}{(2m)!} (\alpha_1^2)^m \right] = 1 - (\alpha_1^2) + \frac{(\alpha_1^2)^3}{3} - \frac{2(\alpha_1^2)^5}{45} + \ldots
\]
\tag{20}
\]

The oscillating sign of these terms is characteristic of the higher-order classes in converging to the true expression. To overcome the unphysicality of \( \mathcal{F}_{\mathcal{O}(1)} \) as the noise content increases we employ a metric \( \mathcal{F}_\chi \) with the physically reasonable properties that
\[
\mathcal{F}_{\text{av}} \approx \mathcal{F}_{\mathcal{O}(1)} \approx \mathcal{F}_\chi, \quad (\alpha_1^2) \ll 1 \tag{22}
\]
\[
\mathcal{F}_{\mathcal{O}(1)} \leq \mathcal{F}_{\text{av}} \leq \mathcal{F}_\chi, \quad (\alpha_1^2) \approx 1 \tag{23}
\]
\[
\mathcal{F}_\chi \to 1/2 \to P_1(\tau), \quad (\alpha_1^2) \gg 1 \tag{24}
\]

We may satisfy these conditions by noticing the qualitative resemblance between Eqs. 20 and 21 and the expansion for a simple exponential
\[
1 - (\alpha_1^2) + \frac{2(\alpha_1^2)^3}{3} + \ldots = \frac{1}{2} \left[ 1 + \sum_{m=0}^{\infty} (-1)^m \frac{2^{2m}}{(2m)!} (\alpha_1^2)^m \right] = \frac{1}{2} \left[ 1 + \sum_{k=0}^{\infty} \left( -\frac{\chi(\tau)}{m!} \right)^m \right] \tag{25}
\]
\[
\text{where we have defined } \chi(\tau) \equiv 2(\alpha_1^2). \text{ Hence we use the following metric in calculating fidelities to be compared with experimental data}
\]
\[
\mathcal{F}_\chi = \frac{1}{2} \left\{ 1 + \exp[-\chi(\tau)] \right\} \tag{27}
\]

This approximation represents the first-order fidelity approximation: it ignores higher-order cross correlations in the noise arising from higher-order Magnus contributions to the error vector, with diminishing overall magnitude (as given by the smallness parameter), but incorporates an approximation to higher-order terms important as the total noise-induced infidelity grows. We work in this limit throughout this manuscript.

**Breakdown of the first-order fidelity approximation**

As described above, the first-order fidelity ignores higher-order terms expressed as nested-integrals over cross-correlations between noise along different directions, assuming weak noise. As these contributions to gate infidelity grow in importance (for instance with \( \alpha \)) we expect the filter-transfer-function fidelity calculations to underestimate measured error in cases where the control has filtered the noise to leading order.

We measure the probability that a \( \pi_2 \)-pulse drives qubit population from the dark state to the bright state, \( |0\rangle \to |1\rangle \), as a function of the high-frequency cutoff, \( \omega_c \), of a white dephasing bath (Fig. 1b). As the high-frequency cutoff of the noise is increased and fluctuations fast compared to the control are added to the noise power spectrum, \( S_n(\omega) \), errors accumulate reducing the measured fidelity. The value of \( \omega_c \) at which the fidelity drops from near unity decreases as a function of the noise strength, parametrized by \( \alpha \). In all cases for the primitive \( \pi \) pulse the fidelity calculated using the filter transfer function matches the measured data well with no free parameters.

Performance is notably different when studying the four-segment WAMF \( \pi \)-pulse, W1, indicated in Fig. 2b-c of the main text. The WAMF construction provides first-order filtering of time-dependent noise (red line in Fig. 2c) (effectively cancelling terms proportional to \( (\alpha_1^2) \)), but does not provide suppression of higher-order terms in the Magnus expansion for fidelity which grow in importance with noise strength. Unlike data for the primitive gate, as the noise strength increases we observe a growing divergence between the measured fidelity and the fidelity calculated using the filter-transfer functions introduced above assuming a first order approximation (Fig. 1b).

This phenomenon is not a function of total error magnitude, but instead occurs for \( \xi^2 \geq 1 \) (red lines, right axis), a proxy measure indicating that we are not formally able to truncate the series expansion for fidelity at first order and must consider higher-order error contributions [11], including Magnus terms above \( (\alpha_1^2) \). These measurements therefore reveal the efficacy of noise filtering and quantitatively demonstrate the bounds of the first-order fidelity approximation as breakdown routinely occurs near the predicted value \( \xi^2 \geq 1 \). Notably, while formal convergence of this series requires \( \xi^2 \ll 1 \), we find reasonable agreement between experiment and theory up to \( \xi^2 \sim 5 \) (Fig. 1c).

**Time-domain filter order vs. Magnus order**

We may formally indicate the functional dependence of the filter function on the control sequence by writing \( F(\tau \omega) = F(\tau \omega; \Gamma_n) \). Noise filtering (and hence error suppression) corresponds to minimizing the area under the filter transfer function in the spectral region where the noise PSD is non-negligible. We therefore define a cost function over a user-defined frequency band which may take the form
\[
A(\Gamma_n) := \int_{\omega_{c1}}^{\omega_{c2}} d\omega F(\tau \omega; \Gamma_n) \tag{28}
\]

to diagnose the filtering effectiveness achieved by the control sequence \( \Gamma_n \); the smaller the integral \( A(\Gamma_n) \), the more effective the noise filtering in this band. Having
defined control sequences as continuous elements of the corresponding control space, for a given \( n \) we may in principle construct a variational procedure on \( x_n \), to derive “values” of \( \Gamma_n \) satisfying a given cost function.

The filter transfer function may be approximated by a polynomial expression \( F(\omega \tau; \Gamma_n) \propto (\omega \tau)^{2p} \) for some \( p \) near \( \omega \approx 0 \). As \( p \) increases the integral in 28, and hence the infidelity, decreases: the noise in the time domain is then said to be filtered to order \( p - 1 \).

Equivalently stated, a control sequence \( \Gamma_n \in x_n \), filters time-dependent noise to order \( p - 1 \) if \( \Gamma_n \) is a concurrent zero of the first \( p - 1 \) coefficients in the Taylor expansion\(^2\).

\(^2\) This procedure is valid for frequencies sufficiently lower than \( 1/\tau \) (the inverse of the total sequence duration).

The dependence of the expansion coefficients on our control parameters \( \Gamma_n \) has been made explicit, and we include only even powers of \( \omega \tau \) due to the evenness of the filter transfer function. In this case \( A(\Gamma_n) \approx c_{2p}(\Gamma_n) \Gamma_n^{2p+1} \) and the condition that

\[
\frac{A(\Gamma_n)}{c_{2p}(\Gamma_n)} = O\left( \frac{\Gamma_n^{2p+1}}{2p+1} \right)
\]

therefore implies the control sequence \( \Gamma_n \) filters noise to order \( p - 1 \). This effect is visualized through the slope of the filter transfer function in the stopband on a log-log plot (Fig. 2c, main text). A high-order filter has a higher slope in this region, indicating improved suppression of time-dependent noise.

General filter design focuses on a band of interest, permitting spectral response to diverge outside of the spectral region of interest - for instance electrical filters in the microwave may appear transparent in the THz or Hz. Therefore, in addition to the asymptotic, zero-frequency filter order \( (p - 1) \), we introduce a more general metric capable of describing filter performance over an arbitrary spectral band. The local filter order \( (p^* - 1) \) establishes that the filter-transfer function is well approximated by \( F_1 \propto (\omega \tau)^{2p^*} \) over the band \( [\omega_1, \omega_2] \). It is this more narrowly defined metric that is used in most practical filter-design tasks, including those undertaken above.

The performance of filter-order \((p - 1)\) or local filter order \((p^* - 1)\) for time-dependent noise described above must be distinguished from the order of error suppression for quasi-static errors. The latter measure is typically used in NMR literature to the pulse sequences designed to compensate for quasi-static errors. In this regime the time dependence of the dephasing (amplitude) noise fields reduces to constants \( \beta_\mu (\beta_\nu) \) and the Magnus expansion terms \( \Phi^{(DC)}_\mu \) are evaluated strictly as time integrals over ideal control operations scaled by powers of the offset magnitude \( \beta_\mu (\beta_\nu) \). A pulse sequence for which \( \Phi^{(DC)}_\mu = \ldots = \Phi^{(DC)}_{\mu-1} = 0 \) is then said to compensate offset errors to order \( \mu - 1 \). In this case the total error operator satisfies \( \Phi^{(DC)}(\tau) = O(\Phi^{(DC)}) \) and is dominated by the residual error proportional to the \( \mu \)th power in the offset magnitude.

High-order error suppression in the Magnus expansion does not imply high-order time-domain noise filtering. Table I reveals the importance of not conflating these two measures when assessing the performance of a control sequence against static vs stochastic errors. The upper panel compares the two performance measures for some well-known phase-modulated NMR sequences, the naming conventions for which are consistent with the review
Walsh basis functions

We impose physically motivated constraints on the form of $\Gamma_n$ in order to reduce the search to a manageable subspace of $C_n$, and elect to synthesize control sequences from the Walsh basis functions. The set of Walsh functions $w_k : [0,1] \rightarrow \{-1, 1\}$, $k \in \mathbb{N}$ form an orthonormal-complete family of binary-valued square waves defined on the unit interval and are the digital analogues of the sines and cosines in Fourier analysis. Since their formulation in the first half of the twentieth century, Walsh functions have played an important role in scientific and engineering applications. Their development and utilization has been strongly influenced by parallel developments in digital electronics and computer science since the 1960s, with Walsh-type transforms replacing Fourier transforms in a range of engineering applications such as communication, signal processing, image processing, pattern recognition, noise filtering and so forth [14].

We summarize the relevant mathematical details of the Walsh basis, outlining two equivalent representations, Paley ordering and the Hadamard representation, both of which are useful to understand the Walsh control space.

Paley ordering

The Walsh functions are aperiodic and hence do not admit to the unique ordering according to increasing frequency characteristic of the sinusoids in the Fourier basis. by Merrill and Brown [13]. For completeness, in the lower panel we also make the comparison for the novel control sequences derived in this paper.

Later we will return to the question of time-domain filter order and introduce a set of analytic design rules for filter construction based on the characteristics of our selected basis functions - the Walsh functions.

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Paley ordering

The Walsh functions are aperiodic and hence do not admit to the unique ordering according to increasing frequency characteristic of the sinusoids in the Fourier basis.
which any continuously defined basis member \( P_{\mathbf{A} k}(x) \) projects completely onto a digital vector in \( \mathbb{R}^{2^n} \) provided \( m(k) \leq n \), which is true for the \( 2^n \) Paley orders in the set \( k \in \{0, 1, ..., 2^n - 1\} \). Since these vectors have dimension \( 2^n \) and inherit the orthogonality of the \( P_{\mathbf{A} k}(x) \) they therefore form a discrete Walsh basis spanning \( \mathbb{R}^{2^n} \).

Such a projection is clearly possible since the fastest modulation rate in \( P_{\mathbf{A} k}(x) \) derives from the periodicity of \( R_{m(k)}(x) \), which switches sign \( 2^{m(k)} \) times over \( x \in [0, 1] \). The projection then involves partitioning the domain into \( 2^n \) bins and associating the value of \( P_{\mathbf{A} k}(x) \) in the \( j \)th bin to the \( j \)th element \( P_{2^n}^{j(k)} \in \{\pm 1\} \) of the discrete digital vector

\[
P_{2^n}^{j(k)} = \left[ P_1^{j(k)}, P_2^{j(k)}, ..., P_{2^n}^{j(k)} \right]. \tag{33}
\]

Using the so-called Sylvester construction [15], the \( 2^n \)-dimensional Hadamard matrix \( H_{2^n} \) is generated recursively by

\[
H_{2^n} = \begin{bmatrix} H_{2^{n - 1}} & H_{2^{n - 1}} \\ -H_{2^{n - 1}} & H_{2^{n - 1}} \end{bmatrix} = S \otimes n \quad \tag{34}
\]

\[
S = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \quad H_1 = 1 \quad \tag{35}
\]

where \( S \) is the Sylvester matrix, and \( \otimes n \) denotes \( n \geq 1 \) applications of the Kronecker product. In this construction \( P_{2^n}^{j(k)} \) defines the \( i(k) = 1 \) for \( \sum_{j=1}^{m(k)} b_j \) column (row) of \( H_{2^n} \). The orthogonality of the Walsh basis is thereby reflected in the property that \( H_{2^n} H_{2^n}^T = 2^n I \), implying the orthogonality of the Hadamard matrices.

This representation is particularly useful for efficiently constructing Walsh-synthesized waveforms. Consider an arbitrary function \( f(x) = \sum_{k=0}^{N} X_k \mathbf{P}_{\mathbf{A} k}(x) \) synthesized in the Walsh basis where \( N \) sets the highest (Paley) ordered function in the construction. Then, from the above discussion, all Walsh functions in this synthesis projected onto a Hadamard matrix of dimension \( \geq 2^{m(N)} \), with \( M = 2^{m(N)} \) giving the minimal sufficient dimension. A discrete representation of the function \( f(x) \) therefore exists as a projection onto the column space of \( H_M \) by writing

\[
f = H_M \tilde{X}. \tag{36}
\]

The column vector \( \tilde{X} = [ \tilde{X}_1, \tilde{X}_2, ..., \tilde{X}_M ]^T \) contains the reordered Paley amplitudes \( X_k \) reordered under the change of basis map \( i(k) \) specified by \( b \)

\[
\tilde{X}_{i(k)} = \begin{cases} X_k & 0 \leq k \leq N \\ 0 & N < k < M \end{cases}. \tag{37}
\]

The vector \( f = [ f_1, f_2, ..., f_M ]^T \) so generated then represents the piecewise constant structure of \( f(x) \), with \( f_j \) giving the value taken by \( f(x) \) on the \( j \)th of \( M \) equal subintervals partitioning \( x \in [0, 1] \).

Walsh synthesis for amplitude modulated filters

Any square integrable function \( f(x) \) on the interval \([0,1]\) has a unique spectral decomposition in the Walsh basis

\[
f(x) = \sum_{k=0}^{\infty} X_k w_k(x) \quad \mathrel{\iff} X_k := \int_{0}^{1} f(x) w_k(x) dx.
\]

We consider a control regime referred to as single-axis amplitude modulation defined by

\[
\Gamma_k = \{(\tau_l, \theta_l)\}_{l=1}^{n}, \quad \phi_l = \phi_0 \quad \forall l \in \{1, ..., n\} \tag{38}
\]

where the waveform structuring the total angle swept out in each pulse segment, \( \theta_l \), is based on a linear superposition of well-defined square waves known as Walsh functions. We refer to these sequences as Walsh amplitude modulated filters (WAMFs), and speak of searching over the Walsh-modulated control subspace.

Using the above framework, we may efficiently construct arbitrary WAMFs for arbitrary pulse-segment envelopes. We define a time-varying Rabi rate \( \Omega(t), l \in \{1, ..., M\} \) over the time period \( t \in [t_{l-1}, t_l] \) of each segment, \( l \in \{1, ..., M\}, t \in [t_{l-1}, t_l] \). Each segment has duration \( \tau_l = \tau/M \) and generates a total rotation angle for each segment, \( \theta_l \) given by the integral

\[
\theta_l = \int_{t_{l-1}}^{t_l} \Omega(t) dt. \quad \tag{39}
\]

We now treat the rotation angles \( \theta_l \) as parameters by which to optimize filter performance. For efficient filter construction, however, it is convenient to instead transform this optimization over \( \theta_l \) to an optimization over the Walsh spectrum. This is achieved by writing \( \theta_l = \theta_l(X_0, X_1, ..., X_N) \) with the dependence on the Walsh spectra defined by the Hadamard-matrix equation

\[
\bar{\theta} = (\theta_1, \theta_2, ..., \theta_M)^T = (\tau/M) H_M \tilde{X}. \tag{40}
\]

Defined in this way, the \( M\)-segment arbitrary-envelope construction achieves total gate-rotation angle \( \Theta = \sum_{l=1}^{M} \theta_l = X_0 \tau \), completely determined by the spectral amplitude of \( \mathbf{P}_{\mathbf{A} 0} \). All symmetry-based design rules carry over, regardless of the modulation envelope for an individual pulse segment.

Square pulses

The special case of square pulse segments is treated here as it allows a reduction in synthesis complexity and is compatible with many experimental systems. We may replace the time-dependent Rabi rate \( \Omega(t) \) over a single segment with a piecewise-constant (over a single-segment) construction used in Walsh synthesis over a
complete pulse sequence
\[ \Omega(t) = \sum_{k=0}^{N} X_k \text{PAL}_k(t/\tau), \quad t \in [0, \tau]. \] (41)

This permits synthesis over the Rabi rate per segment rather than the total rotation angle, which is often simpler in experimental settings. Substituting \( \Omega(t/\tau) \) for \( f(x) \) in Eq. 36 we obtain \( \Omega = H_M \hat{X} \). The vector \( \Omega = [\Omega_1, \Omega_2, ..., \Omega_M]^T \) thus defines a sequence of modulated Rabi rates each functionally dependent on the Walsh amplitudes
\[ \Omega_l = \Omega_l(X_0, X_1, ..., X_N), \quad l \in \{1, ..., M\}. \] (42)

The WAMF is then defined by explicitly writing \( \Omega \) as an additional column leading the representation of Eq. 5, yielding the form
\[ \Gamma_M = \left[ \begin{array}{cccc}
\Omega_1 & \phi_1 & \theta_1 & \\
\Omega_2 & \phi_2 & \theta_2 & \\
\vdots & \vdots & \vdots & \\
\Omega_M & \phi_M & \theta_M & 
\end{array} \right] \] (43)

Here the degree of freedom associated with \( \tau_l \) has apparently been removed. This reflects the fact that the choice of \( \tau_l \) has been transformed into the choice of Walsh basis functions in the synthesis, each contributing its characteristic temporal profile. The remaining degrees of freedom reside in functional dependence of \( \Omega_l \) on the Walsh spectrum and our variational search is thus limited to the subspace of \( \mathcal{F}_M \), effectively spanned by \( \hat{X} \).

Negative Walsh spectral amplitudes may produce negative valued Rabi rates under a linear superposition. For a pulse of the form \( P_l = \exp \left[ -i \Omega_l \tau_l \phi_l / 2 \right] \) the negative sign of \( \Omega_l \) may be absorbed into the spin operator \( \phi_l \) correspondingly to the application of a \( \pi \) phase shift int he driving field. This follows from the fact that \( \sigma_{\phi,a} = -\sigma_{\phi} \), which is clear from the definition of our spin operator in Eq. 3. Thus including negative-valued Walsh spectral amplitudes generally produces single axis control only up to a sign change.

**Gaussian pulse envelopes**

The square-envelope pulses studied experimentally in the main text are easy to generate in our experimental system but may prove difficult in other settings where abrupt amplitude shifts at timestep-edges produce significant pulse distortion. Here we show that achieving Walsh synthesized filters using a common Gaussian pulse envelope yields comparable results with a simple re-optimization of Walsh-synthesis coefficients.

The square amplitude-modulated waveform is here replaced with a smoothly varying pulse envelope in each segment, each associated with a specific rotation angle \( \theta_l \) subject to optimization. We assume a Gaussian profile \( G_l(t; \mu_l, \sigma_l) \) defined on \( t \in [t_{l-1}, t_l] \) with mean \( \mu_l \) and standard deviation \( \sigma_l \). Specifically, we construct
\[ G_l(t; \mu_l, \sigma_l) = \frac{\theta_l}{C_l \sigma_l \sqrt{2\pi}} \exp \left[ -\frac{(t - \mu_l)^2}{2\sigma_l^2} \right] \] (44)
\[ \mu_l = \frac{t_{l-1} + t_l}{2} \] (45)
\[ \sigma_l = g\tau/M \] (46)

with \( \mu_l \) the segment midpoint and \( \sigma_l \) expressed as a multiple \( g \) of the segment duration. The normalizing factor
\[ C_l := \int_{t_{l-1}}^{t_l} \frac{1}{\sigma_l \sqrt{2\pi}} \exp \left[ -\frac{(t - \mu_l)^2}{2\sigma_l^2} \right] dt \] (47)
is included to ensure the total rotation implemented by the Gaussian pulse in the \( l \)th segment is given by \( \int_{t_{l-1}}^{t_l} G_l(t; \mu_l, \sigma_l) dt = \theta_l \). We now impose the same structure on the segment rotations \( \theta_l \) as presented above in Eq. 40. Defined in this way, the \( M \)-segment Gaussian-pulse sequence shares with the square WAMF construction the property that the total gate rotation angle \( \Theta = \sum_{l=0}^{M} \theta_l = X_M \tau \) is completely determined by the spectral amplitude of PALM.

We may therefore construct a Gaussian-pulse variation on any candidate WAMF such that, having set \( g \) to some value relevant to the control hardware, the smooth pulse sequence remains strictly parametrized in the Walsh spectrum \( X \). In particular, filter optimization proceeds in the same manner as for ordinary Walsh-modulated control by minimizing the cost function with respect to the Walsh spectrum.

**Analytic design rules**

An advantage of Walsh synthesis is that the well-defined spectral properties and symmetries of the Walsh functions may be employed to further restrict the search space available for filter construction.

First, in practice the achievable filter order over the entire stopband is limited by the number of constituent control operations; one may achieve higher \( p \) at the cost of higher \( n \). The maximum achievable value of \( p \) for a given filter is set by the power-law expansion of the filter for the single Walsh function with the highest Paley order for a given \( n \). As has been shown previously, all Walsh functions with given Hamming weight of the Paley order have the same power-law expansion near zero frequency [16]. Therefore, in principle, every doubling of \( n \) increases the maximum achievable time-domain filter order by one. The Walsh functions highlighted in red in
Fig. 2 represent those with the highest Paley-order Ham-
ming weight for a given \( n \). Nonetheless we find that in
general we are able to construct filters with higher order
than prescribed over narrow regions in the stopband, as
a result of Walsh synthesis (see the multiple slopes for
the blue line in Fig. 2c).

In filter construction we may further constrain the form
of a candidate pulse sequence by imposing required phys-
ical properties on the sequence, such as fixing the total
rotation angle of the Bloch vector in order to implement
a target logic operation. In order to proceed we then par-
tition the Walsh spectrum \( \mathbf{X} \equiv (\mathbf{X}_\nu, \mathbf{X}_\rho) \) into spectral
amplitude classes \( \mathbf{X}_\nu \) and \( \mathbf{X}_\rho \) to be treated as vari-
tional and fixed parameters respectively. Fixed param-
ters set the physical state transformation of interest while
the remaining unconstrained components in \( \mathbf{X}_\nu \) serve as
tuning parameters by which to minimize \( A(X_\nu;X_\rho) \).

The primary constraint in WAMF constructions is that
the total rotation angle executed depends only on the
value of \( X_0 \), the zeroth order spectral component; it sets
the effective average Rabi rate for the WAMF. This can
be seen as follows. First observe all Walsh functions of
higher than zeroth order are \( \text{balanced} \) in the sense that
\( \int_0^\tau \text{PAL}_k(x)dx = \delta_{0k} \). For the control field defined by Eq.
41 the total gate rotation angle \( \Theta = \int_0^\tau \Omega(t)dt \) then takes
the form

\[
\Theta = \int_0^\tau \sum_{k=1}^N X_k \text{PAL}_k(t/\tau)dt = \tau \sum_{k=1}^N X_k \int_0^\tau \text{PAL}_k(x)dx
\]

\[
= \tau \sum_{k=1}^N X_k \delta_{0k} = X_0 \tau.
\]

In this case the net gate rotation \( \theta = \Theta \mod 2\pi \) is given by

\[
\theta = X_0 \tau \mod 2\pi \label{eq:48}
\]

implying the necessary constraint on \( X_0 \) in order to
achieve a desired \( \theta \).

Next, we observe that the Walsh functions have dis-
tinct parity, but that filter constructions mandate sym-
metric constructions in order to enact a target operation
and provide effective noise cancellation. The result is
that odd-parity Walsh functions may generally be ex-
cluded from the variational search. While this is not
necessarily strictly required (multiple odd parity Walsh
functions may in principle be added with opposite signs
to produce net symmetric constructions), it is convenient
and effective to restrict the synthesis space to the so-
called CAL subset of the Walsh functions.

Our reduced search problem may then be represented
formally by replacing \( \mathbf{Y}_M \rightarrow (\mathbf{X}_\nu, \mathbf{X}_\rho) \) in Eq. 28 to
obtain

\[
A(X_\nu;X_\rho) := \int_0^\tau d\omega \mathcal{F}(\tau\omega;X_\nu,X_\rho) \label{eq:49}
\]

with the variational search now restricted to the subspace
spanned by \( X_\nu \) with the \( X_\rho \) held constant.

**First order WAMFs**

As a first application of the above result, we derive a
family of nontrivial gates decoupled to first order against
dehasing noise by constructing a pulse sequence from
the synthesis \( \theta(t) = \frac{\pi}{\tau} \left( X_0 \text{PAL}_0(t/\tau) + X_3 \text{PAL}_3(t/\tau) \right) \). Note
that \( \theta(t) \) is only formally defined at the end of
pulse segments. That is, we set \( X_\nu \equiv X_0 \) and \( X_\nu \equiv X_3 \). In this case \( N = 3 \) and \( M = 4 \), so the
minimal pulse duration is \( \tau/4 \). Using Eq. 37 we ob-
tain \( X = \left[ X_1, X_2, X_3, X_4 \right]^T \) as
yielding the minimal Hadamard representation

\[
\theta = \frac{\tau}{4} \begin{bmatrix}
1 & 1 & 1 & 1 \\
-1 & -1 & -1 & -1 \\
1 & 1 & -1 & 1 \\
-1 & -1 & 1 & 1
\end{bmatrix}
\left[ \begin{array}
X_0 \\
X_1 \\
X_2 \\
X_3
\end{array} \right] = \frac{\tau}{4} \left[ \begin{array}
X_0 + X_3 \\
X_0 - X_3 \\
X_0 - X_3 \\
X_0 + X_3
\end{array} \right] \label{eq:50}
\]

These sequences therefore span the control subspace
parametrized by \( \tau = 1 \)

\[
\begin{array}
\Omega_1 & \phi_1 & \phi_2 \\
\rho_1 & X_1 & X_2 & X_3 & X_4 & 0 \\
\rho_2 & X_1 & X_2 & X_3 & X_4 & 0 \\
\rho_3 & X_1 & X_2 & X_3 & X_4 & 0 \\
\rho_4 & X_1 & X_2 & X_3 & X_4 & 0
\end{array}
\]

WAMF \( \mathcal{O}(1) \) =

where we have defined \( X_4 = X_0 + X_3 \). This choice is moti-
vated by the fact that Paley order \( k = 3 \) corresponds to
the lowest order non-constant Walsh function with even
symmetry about \( \tau/2 \) (Fig. 2). Hence 50 is the sim-
plest Walsh modulated form which includes the zeroth
order Walsh function in the synthesis and which pos-
sesses time-reversal symmetry about the sequence mid-
point. The former property ensures a nontrivial gate
angle is executed. The latter is chosen due to the ob-
servation in dynamic decoupling literature that using
time-symmetric building blocks often improves the per-
formance of the sequence compared to sequences formed
by time-asymmetric building blocks[17][18]. In this con-
struction we have maintained a leading column of rabi
rates, \( \Omega_1 \), as would be appropriate for the square-pulse
forms used in the main text.
Gaussian pulse construction

Adding to the results presented in the main text, constructing the 4-segment filter $W1$ using square pulse segments, we examine the Gaussian-pulse variation here. The cost function $A_x(X; X_0)$ may be computed by partitioning the time domain into a large number $N_x$ of subintervals on which the continuous Gaussian envelope is treated as approximately constant. Fig. 3 shows a two-dimensional representation of $A_1(X; X_0)$ integrated over the interval $\omega \in [10^{-2}, 10^{-6}] \tau^{-1}$, with $g = 1/6$ and $N_x = 100$. The value of $\log_{10}(A_1(X; X_0))$ is indicated by the color scale. Total sequence length is normalized to $\tau = 1$ in this data, so the total gate rotation angle $\Theta \equiv X_0$ is given directly by the $X_0$-axis. Regions in blue represent effective (first-order) filter constructions, where the cost function is minimized.

We conclude useful filter construction using Gaussian pulses is a simple matter of re-optimization in the Walsh-synthesis framework. This is readily achieved using a Nelder-Mead optimization of $A_3(X; X_0)$ for any particular choice of $g, \omega, \tau, X_0$ or $N_x$ in a manner precisely the same as for square envelopes.

Universal Filters by Concatenation

Phase-modulated sequences robust against amplitude noise may also be found in the Walsh basis, yielding Walsh phase-modulated filters (WPMFs) analogous to WAMFs, and implementing arbitrary target rotations $\theta$. There are a variety of techniques to construct such WPMFs, but we use analytic design rules in which a target rotation is performed (with some error due to noise), and phase-modulated segments are added in order to produce the net filtering effect. The simplest WPMF adds two segments phase modulated according to Walsh function $PAL_4$ with coefficient $X_1$, subject to the constraint that one enacts the desired driven rotation by $\theta$.

The result of this approach yields a WPMF that is identical to the NMR sequence $SK1$, with value $X_1 = \cos^{-1}(-\theta/4\pi) \equiv \phi_{SK1}(\theta)$ [13], as represented

\[
\begin{bmatrix}
\Omega_0 & \theta & \tau_0 & \phi_0 \\
\Omega_0 & \theta & \tau_\phi & \phi_{SK}
\end{bmatrix}
\]

\[
\begin{bmatrix}
\Omega_0 & 2\pi & \tau_2 & \phi_{SK1} \\
\Omega_0 & 2\pi & \tau_2 & -\phi_{SK1}
\end{bmatrix}
\]

\[
\Omega_0 = \frac{\theta + 4\pi}{\tau}, \quad \tau_0 = \frac{\theta}{\Omega_0}, \quad \phi_{SK1}(\theta) = \cos^{-1}\left(-\frac{\theta}{4\pi}\right).
\]

Note that the Walsh timing construction only holds in the two correction steps represented above. Following a similar route allows one to construct a sequence with modulation given by $PAL_3$ which is formally identical to the three-segment (four-timestep) phase modulation given by gate $P2$ [13].

These WPMF sequences perform as first-order time-dependent noise filters, captured in the form of $F_{\Omega}(\tau\omega)$, and noted in Table 1 (column 2). For example, filter functions for the WPMF that is equivalent to $SK1$ are shown in Fig. 4b, revealing first-order filtering of amplitude noise, but not dephasing noise.

We may now concatenate WAMFs and WPMFs in order to simultaneously filter universal noise. We focus on an explicit example providing first-order amplitude and dephasing noise filtering. The basic procedure is to implement each constant-amplitude segment of a four-segment WAMP $W1$, using a constant-amplitude phase-modulated sequence robust against amplitude noise. As a reminder, the noise-filtering performance of $W1$ is shown in Fig. 4c. Here we use the WPMF$\equiv SK1$ sequence for
the phase modulation. We refer to the concatenated gate as a Universal Walsh Modulated Gate, UWMF$_{1,SK1}$.

Referring to Eq. 51, the WAMF filter is similarly written $P_3(X_+/4, 0)P_2(X_-/2, 0)P_1(X_+/4, 0)$. Concatenation then involves the operator substitutions

$$P_1(X_+/4, 0) \rightarrow \text{SK1}^{(1)}(X_+/4)$$  \hfill (54)

$$P_2(X_-/2, 0) \rightarrow \text{SK1}^{(2)}(X_-/2)$$  \hfill (55)

$$P_3(X_+/4, 0) \rightarrow \text{SK1}^{(3)}(X_+/4).$$  \hfill (56)

The composite structure for UWMF$_{1,SK1}$ is shown in Fig. 4a. Here the SK1 phase flips $\phi = \pm \phi_{SK1}$ within each segment of the WAMF profile are indicated by the oppositely oriented hatching; $\phi = 0$ is indicated by white fill. The dephasing and amplitude filter functions for the concatenated sequence are shown in Fig. 4d, indicating effective filtering of both amplitude and dephasing noise.

**Ytterbium Ion Trapping**

We use trapped $^{171}$Yb$^+$ ions as our experimental platform; a detailed description of related experimental approaches appears in [19, 20]. A linear Paul trap enclosed in an ultra-high vacuum (UHV) chamber is used to trap several hundred $^{171}$Yb$^+$ ions as a small homogeneous ensemble (in magnetic field and microwave field amplitude). Doppler cooling of the ions is achieved using 369 nm laser light, slightly red-detuned from the $^2S_{1/2}$ to $^2P_{1/2}$ transition. Additional lasers near 935 nm and 638 nm are employed to depopulate metastable states.

Our qubit is the 12.6 GHz hyperfine splitting between the $^2S_{1/2}$ $|F = 0, m_f = 0\rangle$ and $^2S_{1/2}$ $|F = 1, m_f = 0\rangle$ states. For notational simplicity we will designate $|0\rangle$ and $|1\rangle$ to these states respectively. Addition of a 2.1 GHz sideband to the 369nm laser using an electro-optic modulator permits high-fidelity state preparation in $|0\rangle$. For details of ion loading, laser cooling, state preparation, and state detection see [20]. While we typically employ a small ensemble of ions, the system behaves similarly to single-ion experiments in our lab, and benefits from both high-fidelity state initialization and projective measurement - the system does not bear similarity to NMR-style ensembles.

State detection is achieved by counting 369 nm photons scattered from the ions and converting to a probability that the Bloch vector lies at a particular location along a meridian of the Bloch sphere. This measurement is susceptible ion loss in the ensemble and both laser amplitude and frequency drifts over long timescales, resulting in variable maximum and dark count rates over time. We therefore employ a normalization and Bayesian estimation procedure for state detection, see [20].

An important advantage of this system is that the selected qubit transition is first order insensitive to magnetic field fluctuations; the measured free-evolution in our setup is $T_2 \approx 4$ s, limited by coherence between the qubit and the master oscillator [20]. Coherent rotations between the measurement basis states are driven by using the magnetic field component of resonant microwave radiation. The Rabi rate for driven oscillations reaches $\sim 14$ µs in our system, with typical operation near $\sim 50$ µs. Rotations are implemented about an axis $\vec{r}$ lying on the $xy$-plane of the Bloch sphere and set by the phase of the microwaves as $\vec{r} = (\cos \phi(t), \sin \phi(t), 0)$. Driven operations, characterized by randomized benchmarking, exhibit a mean fidelity in excess of 99.99%.

**Noise Engineering**

In the laboratory we rely on engineering noise in our control system to provide a method to accurately reproduce decoherence processes of interest. We begin with a desired noise power spectral density in either the amplitude or detuning quadrature (or both), assuming they are statistically independent. From this power spectrum, defined by the noise strength $\alpha$, the exponent of the power-law scaling $p$, the comb spacing $\omega_0$, and the high-frequency cutoff $\omega_c \geq J_\omega$, we numerically generate time-domain vectors for amplitude and frequency errors. Noise is injected into the system by adding these modulation patterns on top of the control sequence being implemented (e.g. a pulse of radiation for implementing a $\pi$-pulse) using IQ modulation in our vector signal generator [20].
Randomized Benchmarking

We use randomized benchmarking as a tool for resolving small gate errors which cannot be resolved in the application of a single gate. Our randomized benchmarking sequence consists of interleaved $\pi/2$ and $\pi$ pulses each applied along axes randomly selected from $\pm x$ and $\pm y$. Each sequential pair of $\pi/2$ and $\pi$ rotations is referred to a computational gate. A given randomized benchmarking sequence consists of $l$ computational gates followed by a final correcting gate which is selected such that the aggregate Unitary operation applied is a $\pi$ rotation. For each $l$ we measure 50 randomizations (dots in Fig. 3f of the main text), and in each randomization average over 20 different realizations of a white dephasing noise bath. Each realization, in turn, employs 20 measurements in our Bayesian state-detection algorithm, in addition to associated normalization experiments.

Comparisons of W1 to primitive $\pi$ rotation performance in randomized benchmarking is conducted via replacement of all $\pi$ pulses with W1 constructions, again about randomly selected axes. In either case the $\pi/2$ rotation is achieved using a primitive gate, although we have also validated that replacement of the $\pi/2$ gates with WAMF constructions yields net improvement in gate fidelity.

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Appendix B

*Physical Review A* publication
Experimental bath engineering for quantitative studies of quantum control

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We develop and demonstrate a technique to engineer universal unitary baths in quantum systems. Using the correspondence between unitary decoherence due to ambient environmental noise and errors in a control system for quantum bits, we show how a wide variety of relevant classical error models may be realized through in-phase or in-quadrature modulation on a vector signal generator producing a resonant carrier signal. We demonstrate our approach through high-bandwidth modulation of the 12.6-GHz carrier appropriate for trapped $^{171}\text{Yb}^+$ ions. Experiments demonstrate the reduction of coherent lifetime in the system in the presence of both engineered dephasing noise during free evolution and engineered amplitude noise during driven operations. In both cases, the observed reduction of coherent lifetimes matches well with quantitative models described herein. These techniques form the basis of a toolkit for quantitative tests of quantum control protocols, helping experimentalists characterize the performance of their quantum coherent systems.

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I. INTRODUCTION

The discipline of quantum control engineering [1–4] is addressing pressing challenges in the fields of quantum physics, quantum information, and quantum engineering, attempting to provide the community with a broad range of novel capabilities in the precise manipulation of quantum systems [5–9]. For instance, protocols derived from open-loop control employing sequences of SU(2) operations, known collectively as dynamical decoupling, have proven useful in extending the coherent lifetime of qubits in quantum memories [10–13] and in producing effective noise filters for quantum sensors [14–18].

Beginning with the work of Kurizki et al. [19,20], there has been a substantial effort in the field towards incorporating filter-transfer functions into the vernacular of quantum control [21,22]. This has extended from trivial application of the identity in dynamical decoupling [10,23–27] to arbitrary single- [28–31] and two-qubit operations [32,33]. In this framework, a metric of interest, generally an ensemble-averaged operational fidelity, may be simply calculated from the product of the environmental noise power spectrum and a filter transfer function capturing the effects of the control in the Fourier domain. This approach has been shown to be a general and efficient approach capturing arbitrary control and arbitrary universal noise in quantum systems [30] and is a powerful tool for understanding the influence of realistic colored classical noise power spectra on quantum systems.

These advances are providing a means for theoretical researchers to move away from the unphysical Markovian assumptions for stochastic, uncorrelated error models selected for convenience in quantum error correction and the like [34,35], and has provided a simple platform for the development of novel protocols aimed at improving control fidelity in quantum systems. As these protocols transition from theoretical concepts into the laboratory, experimentalists require techniques to quantitatively verify the predicted performance in different noise environments and compare outcomes in a manner that is insensitive to underlying imperfections in their hardware. Such precise validations are necessary for researchers to confidently develop quantum control techniques using substantiated methodologies and subroutines.

In this paper, we describe a technique to engineer arbitrary unitary baths consisting of dephasing and amplitude-damping processes for quantitative tests of experimental quantum control. We present a simple theoretical model for approximating arbitrary classical power spectra via discrete frequency combs with user-selected envelopes (e.g., $1/f$). We describe how this model permits simple and verifiable creation of time-dependent noise realizations in both dephasing and amplitude-damping quadratures, compatible with experimental systems. Through demonstration of the isomorphism of unitary control errors and environmental decoherence, we map these noise realizations to modulation of a carrier signal in an experimental control system, e.g., for a single quantum bit. Using trapped $^{171}\text{Yb}^+$ ions with splitting $\sim$12.6 GHz, we demonstrate our bath engineering approaches via $IQ$ modulation on the microwave carrier. Ramsey spectroscopy measurements quantitatively verify the predicted influence of engineered dephasing noise on the coherent lifetime of our qubits.

The remainder of this paper is structured as follows. In Sec. 2, we provide a detailed theoretical derivation of our selected method of unitary noise engineering for both dephasing (detuning) and amplitude-damping Hamiltonians, and describe how these noise spectra may be translated to widely available time-domain $IQ$-modulation waveforms applied to a carrier signal. We then move on to describe our experimental system and its capabilities in Sec. 4A. This is followed in Sec. 4 by a characterization of an experimentally implemented noise-engineered bath through direct examination of the carrier and a demonstration of engineered dephasing environments via measurements of coherent lifetimes for $^{171}\text{Yb}^+$ ion qubits. The paper concludes with a discussion and outlook towards future experiments.

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II. PHYSICAL SETTING

In many quantum systems of interest we may consider two general classes of unitary time-dependent errors. Dephasing processes are associated with rotations about \( \hat{\gamma} \) induced by a stochastic relative detuning between a qubit’s transition (angular) frequency \( \omega_\text{r} \) and the experiment’s master clock, defined by a local oscillator (LO). Dephasing is frequently dominated by instabilities in the qubit splitting caused by environmental (e.g., magnetic field) fluctuations. However, in the limit of very stable qubits (e.g., clock transitions in atomic systems [36,37]), observed dephasing may be caused by frequency instabilities in the experimental LO. Similarly, one may consider coherent amplitude-damping processes, causing unwanted rotations along meridians of the Bloch sphere, and arising either through ambient environmental fluctuations (e.g., microwave leakage from nearby systems) or from imperfections in the amplitude of the applied control field.

Together, these two classes of error capture so-called universal (multi-axis) rotations of the Bloch sphere. Importantly, the consideration of time-dependent errors in both dephasing and amplitude quadratures allows us to capture the dominant forms of non-Markovian noise processes characterized by the presence of long-time correlations; realistic laboratory settings are typically dominated by such noise terms. Dissipative error pathways with Markovian characteristics may be captured through linearly independent error terms that we ignore through this treatment, as quantum control generally provides no relevant benefits in error resistance for these effects.

We consider a model quantum system consisting of an ensemble of identically prepared noninteracting qubits immersed in a weakly interacting noise bath and driven by an external control device. Working in the interaction picture with respect to the qubit splitting, state transformations are represented as unitary rotations of the Bloch vector. Including both control and noisy interactions, we may therefore write the generalized time-dependent Hamiltonian

\[
H(t) = H_\text{c}(t) + H_\text{N}(t).
\]  

The term \( H_\text{c}(t) = h(t)\sigma \) represents perfect control over the qubit state via the application of an external field, while the generalized noise term \( H_\text{N}(t) = \eta(t)\sigma \) captures all interactions due to the noise bath. Here, \( \sigma \) denotes a column vector of Pauli matrices and the row vectors \( h(t), \eta(t) \in \mathbb{R}^3 \) denote, respectively, the Cartesian components of the control and noise fields in the basis of Pauli operators [29,30,38]. The stochastic noise fields \( \eta_i(t), i \in \{x,y,z\}, \) model semiclassical time-dependent error processes in each of the three spatial directions. In this formulation, dephasing processes are captured through the appearance of stochastic terms along \( \hat{\gamma} \). General coherent amplitude-damping terms on the other hand are captured by terms proportional to the spin operator \( \hat{\sigma}_\phi := \cos(\phi)\hat{\sigma}_z + \sin(\phi)\hat{\sigma}_x \) parametrized by the driving phase \( \phi \in [0,2\pi] \).

Our choice to write separate control and noise terms in the Hamiltonian in Eq. (2.1) belies the fact that, when expressed in an appropriate interaction picture, time-dependent fluctuations in either term are effectively indistinguishable. This observation permits a formulation in which the noise terms are all incorporated into the control Hamiltonian, and one assumes the presence of a perfectly stable qubit (i.e., there is no ambient decoherence). This is a good approximation in the case of a sufficiently stable qubit so long as native error rates and ambient noise susceptibilities are small compared to relevant scales under study. We therefore proceed by providing a model for quantum dynamics that permits us to capture unitary decoherence through the control.

With these generalized notions in mind, we proceed in laying out the detailed Hamiltonian framework relevant to our study. The system considered in this paper consists of a qubit with transition (angular) frequency \( \omega_\text{r} \), driven by a LO with magnetic field component aligned with \( \hat{\gamma} \) taking the form

\[
\eta(t) = \Omega(t) \cos(\omega_\text{r}t + \phi(t))\hat{\gamma},
\]

\[
\Omega(t) = \Omega_C(t) + \Omega_N(t),
\]

\[
\phi(t) = \phi_C(t) + \phi_N(t)
\]

with \( \omega_\text{r} \) the carrier frequency. In this formulation, the time dependence of the phase \( \phi(t) \) and amplitude \( \Omega(t) \) has been formally partitioned into components denoted by the subscripts \( C \) and \( N \), capturing the desired control and noisy interactions, respectively. Using standard approximations, and working in an interaction picture (see Appendix A), the system Hamiltonian (\( \hbar = 1 \)) may be expressed as

\[
H_I = -\frac{\phi_C(t)}{2}\hat{\sigma}_z + \frac{1}{2}\Omega(t)[\cos(\phi_C(t))\hat{\sigma}_z + \sin(\phi_C(t))\hat{\sigma}_x].
\]

The noise component \( \phi_N(t) \) of the engineered phase \( \phi(t) \) produces net rotations about \( \hat{\gamma} \) through its time derivative \( \phi_N(t) \), and the resonant carrier field drives coherent Rabi flopping between the qubit states \( |1 \rangle \) and \( |0 \rangle \). The instantaneous Rabi rate in this case is proportional to \( \Omega(t) \), and rotations, generated by the spin operator \( \hat{\sigma}_\phi(t) \), are driven about the axis \( \vec{r} = [\cos(\phi(t)), \sin(\phi(t)),0] \) in the \( xy \) plane of the Bloch sphere.

Given sufficient control over both the phase and amplitude of our driving field, Eq. (2.5) therefore indicates we may engineer a variety of effective control Hamiltonians with dephasing and amplitude-damping terms of interest. For instance, setting \( \phi_C(t) = 0 \), we may generate

\[
H(t) \propto \begin{cases} h_z(t)(1 + \eta_z(t))\hat{\sigma}_z & \text{(Mult. Amp. Noise),} \\ h_x(t)(1 + \eta_x(t))\hat{\sigma}_x & \text{(Add. Amp. Noise),} \\ \eta_x(t)\hat{\sigma}_x + \eta_z(t)\hat{\sigma}_z & \text{(Add. Deph. Noise),} \\ \end{cases}
\]

where the control field \( h_z(t) \) is proportional to \( \Omega_C(t) \) and the noise fields \( \eta_x(t) \) or \( \eta_z(t) \) may be switched on, with desired spectral properties, by an appropriate choice of \( \Omega_N(t) \) and \( \phi_N(t) \), respectively.

The Hamiltonians in Eq. (2.6) correspond to familiar error models from NMR and quantum information [39,40], but now explicitly incorporate non-Markovian time-dependent effects through the power spectra of the relevant terms in \( \eta(t) \). The first noise model may be produced in the absence of Hamiltonian
terms that look like $h_x(t)\eta_x(t)$ by virtue of the ability to arbitrarily parametrize $\eta_x(h_x(t), t)$.

Following previous work, we express the first-order averaged fidelity of an arbitrary unitary control operation on SU(2) in the presence of noise as [30]

$$F_{\text{av}}(\tau) \approx \frac{1}{2} [1 + \exp\{-\chi(\tau)\}], \quad (2.7)$$

$$\chi(\tau) = \frac{2}{\pi} \int_0^\infty \frac{d\omega}{\omega^2} S_\psi(\omega) F_\psi(\omega) + \int_0^\infty \frac{d\omega}{\omega^2} S_\psi(\omega) F_\psi(\omega)^* . \quad (2.8)$$

Here, we have defined independent noise power spectra $S_\psi(\omega)$ and $S_\psi(\omega)$, with angular frequency $\omega$, for fluctuations in $\phi_\psi(t)$ and $\Omega_\psi(t)$, respectively, while the quantities $F_\psi(\omega)$ and $F_\psi(\omega)$ represent the spectral characteristics of the control under study. While we will not focus on the particular form of this so-called filter transfer function expression for operational fidelity [28,30], we can clearly see the importance of these noise power spectra in determining the performance of an arbitrary control operation. Consequently, in the following section, we derive their forms.

III. ENGINEERING NOISE IN THE CONTROL SYSTEM

In the laboratory we rely on engineering noise in our control system to provide a method to accurately reproduce decoherence processes of interest. This approach has significant benefits over, e.g., noise injection in ambient magnetic field coils, as it minimizes potential nonlinearities and frequency-dependent responses in hardware elements, exploiting instead the modulation capabilities of a carrier synthesis system [41]. By engineering noise through a highly accurate control system with linear response, we gain the ability to perform quantitative tests of quantum control in the presence of unitary noise Hamiltonians.

We employ the phase- and amplitude-modulation capabilities in state-of-the-art quantum control systems in order to provide access to the error models of interest. In the remainder of this section, we present a mathematical formalism linking our error model in the geometric picture of unitary dynamics to the properties of a near-resonant drive field of the form given in Eq. (2.2).

A. Arbitrary dephasing (detuning) power spectra

We begin with the case of noise proportional to $\delta_\tau$. Our method relies on generating stochastic detuning errors by performing phase modulation on a constant-amplitude carrier, thereby implementing an effective pure dephasing Hamiltonian. Setting $\Omega_\psi(t) = \phi_c = 0$ and $\Omega_\psi = \Omega_\psi$ we write

$$B(t) = \Omega_\psi \cos[\omega_\psi t + \phi_x(t)] 2 \quad (3.1)$$

$$\phi_n(t) = \alpha \sum_{j=1}^J F(j) \sin(\omega_j t + \psi_j) \quad (3.2)$$

where $\psi_j$ is a random number. That is, the driving carrier tone is modulated to include a time-dependent, stochastic error in the phase constructed as a discrete Fourier series with a base frequency $\omega_\psi = \omega_0/2\pi$, with $\alpha$ being a global scaling factor [42].

The link between this phase modulation and the dephasing power-spectral density of interest is revealed by defining the instantaneous phase in terms of the carrier plus a time-dependent detuning $\beta_i(t)$:

$$\Phi(t) = \Phi_0 + \int_0^t dt' \omega_{\psi} + \beta_i(t') \quad (3.3)$$

where $\beta_i(t)$ is a zero-mean time-dependent random variable. This then implies

$$\phi_n(t) = \Phi_0 + \int_0^t d\tau \beta_i(\tau) \quad (3.4)$$

so the time-dependent detuning noise $\beta_i(t)$ is explicitly linked to the phase modulation of the carrier, characterizes the strength of the dephasing-noise term in Eq. (2.5).

Using the Euler decomposition, we may then write

$$\beta_i(t) = \frac{\alpha \omega_\psi}{2} \sum_{j=1}^J F(j)[e^{i(\omega_j t + \psi_j)} + e^{-i(\omega_j t + \psi_j)}] \quad (3.5)$$

Assuming wide-sense stationarity, the two-time correlation function for $\beta_i(t)$ is then written

$$\langle \beta_i(t + \tau) \beta_i(t) \rangle = \frac{\alpha^2 \omega_\psi^2}{2} \sum_{j=1}^J |F(j)|^2 \cos(\omega_j \tau) \quad (3.6)$$

where $\langle \ldots \rangle$ denotes averaging over all times $t$ from which the relative lag of duration $\tau$ is defined. Invoking the Wiener-Khintchine theorem [43] and moving to the Fourier domain, we then obtain the power-spectral density

$$S_i(\omega) = \frac{\pi \alpha^2 \omega_\psi^2}{2} \sum_{j=1}^J |F(j)|^2 \delta(\omega - \omega_j) + \delta(\omega + \omega_j) \quad (3.7)$$

The detailed derivation of the above expressions appears in Appendix B.

The power-spectral density (PSD) is thus represented as a Dirac comb of discrete frequency components with the amplitude of the $j$th tooth determined by the quantity $|F(j)|^2$. We now have an explicit relationship between an effective dephasing- or frequency-detuning -noise power spectrum and the phase modulation of the carrier frequency in the control system required to achieve that PSD.

It is then straightforward to specify the construction of any power-law PSD by writing the amplitude of the $j$th frequency component as a power law $S_i(\omega) \propto (\omega^0)^p$. It therefore follows that the envelope function for the comb teeth in the phase modulation scales as

$$F(j) = j^{\frac{1}{p} - 1} \quad (3.8)$$

Table I shows the functional form required for $F(j)$ in order to achieve dephasing-noise PSDs of interest.
**TABLE I. Functional form of $F(j)$ for well-known dephasing- and amplitude-noise PSDs.**

<table>
<thead>
<tr>
<th>Dephasing</th>
<th>Amplitude</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1/j^2$</td>
<td>$1/f$</td>
</tr>
<tr>
<td>$1/j^2$</td>
<td>$1/f$</td>
</tr>
<tr>
<td>$p$</td>
<td>$F(j)$</td>
</tr>
<tr>
<td>$j^{-2}$</td>
<td>$j^{-3/2}$</td>
</tr>
<tr>
<td>$j^{-1}$</td>
<td>$j^{-1/2}$</td>
</tr>
<tr>
<td>$j^{1/2}$</td>
<td>$j^{1/2}$</td>
</tr>
</tbody>
</table>

**B. Arbitrary amplitude power spectra**

Derivation of the relevant amplitude noise power spectra proceeds in a similar manner. We consider here multiplicative amplitude noise, although the derivation maintains a similar form in the case of additive noise. Further, in our model the amplitude noise is always assumed to be coaxial with the driving field. While this is not a strict requirement, it greatly simplifies the analysis and broadly represents an interesting class of time-dependent error models incorporating driving-field noise. The relevant modulation capability here is, as expected, amplitude modulation on a carrier signal. Setting $\phi(t) = 0$, $\Omega_0(t) = \Omega_0$, and $\Omega_N = \Omega_0 \beta_j(t)$, Eq. (2.2) reduces to

$$B(t) = \{\Omega_0[1 + \beta_j(t)]\} \cos(\omega_0 t) \hat{\mathbf{z}}. \quad (3.9)$$

That is, amplitude modulation transforms the control field strength as

$$\Omega_0 \rightarrow \Omega_0[1 + \beta_j(t)], \quad (3.10)$$

where, again, $\beta_j(t)$ is a zero-mean stochastic random variable here capturing fluctuations in the drive amplitude. This term is realized directly through the comb of discrete frequency components with randomly selected phase shifts

$$\beta_j(t) = \alpha \sum_{j=1}^{J} F(j) \cos(\omega_j t + \psi_j) \quad (3.11)$$

$$= \alpha \sum_{j=1}^{J} F(j)[e^{i(\omega_0 t + \psi_j)} + e^{-i(\omega_0 t + \psi_j)}]. \quad (3.12)$$

The form of this expression is similar to that above for dephasing noise, except the direct-amplitude modulation removes a factor of $j$ from the expression. We are interested in producing a PSD for the quantity $\beta_j(t)$ as this captures the amplitude errors pertaining to the second term of Eq. (2.8). Following the same method as before (see Appendix B), we obtain

$$S_{\alpha}(\omega) = \frac{\alpha^2}{2} \sum_{j=1}^{J} F(j)^2[\delta(\omega - \omega_j) + \delta(\omega + \omega_j)]. \quad (3.13)$$

Once again, we may define a relationship between the power law of the target noise power-spectral density and the quantity $[F(j)]^2$, which determines the amplitude of the $j$th tooth in the frequency comb PSD above. In this instance, the removal of a differential relationship between the modulation and desired noise power spectrum yields the simplified expression $F(j) = j^{p/2}$ for $S_{\alpha}(\omega_0) \propto (\omega_0 t)^p$.

**C. Summary**

With these relationships, we now have explicit links between the quantities we wish to engineer in realizing unitary dephasing or relaxation noise power spectra and the relevant parameters entering into the modulation of a control signal. We will employ these relations to engineer arbitrary unitary noise baths for quantitative tests of various quantum control protocols.

In implementing bath engineering in the laboratory, we are left with the following free parameters:

(i) $\omega_0$: the quadrature of noise injection (dephasing vs amplitude);
(ii) $\Omega_0$: the fundamental frequency of the Dirac comb and the lower cutoff of the noise power spectrum;
(iii) $J$: the maximum number of comb teeth in the discrete sum, setting the upper frequency cutoff $J\omega_0$;
(iv) $p$: the exponent setting the frequency dependence of the effective noise power spectrum.

These parameters provide an experimentalist with a broad set of capabilities for bath engineering (see Table I and Fig. 1).

**IV. EXPERIMENTAL BATH ENGINEERING**

A. **Experimental platform**

The approach we have described above is quite generic for the case of a quantum system controlled by an oscillatory signal, including most atomic, superconducting, and many semiconductor-based spin qubits. In this section, we describe the experimental platform we will employ for validation of our method.

We use trapped $^{171}$Yb$^+$ ions as our model experimental platform; a detailed description of related experimental approaches appears in [37]. Neutral $^{171}$Yb is ionized using a two-photon process whereby 399-nm light excites electrons from $^1$S$_0$ to $^1P_1$ and 369-nm light is sufficiently energetic to further excite electrons to the continuum. A linear Paul trap enclosed in an ultrahigh vacuum (UHV) chamber is used to trap several hundred $^{171}$Yb$^+$ ions. Doppler cooling of the ions is achieved using 369-nm laser light, slightly red-detuned from the $^2$S$_{1/2}$ to $^2P_{1/2}$ transition. Additional lasers near 935 and 638 nm are employed to depopulate metastable states. Typical experiments employ ensembles of approximately 100–1000 ions with high homogeneity in magnetic field and microwave field over the ensemble.

Our qubit is the 12.6-GHz hyperfine splitting between the $^2$S$_{1/2}$($F = 0, m_f = 0$) and $^2$P$_{1/2}$($F = 1, m_f = 0$) states. For notational simplicity we denote these states by $|0\rangle$.
and $|1\rangle$ respectively. The system may be optically pumped to $|0\rangle$ using a 2.1-GHz sideband on the 369-nm cooling beam, which couples the states $|S_{1/2}F=1\rangle \leftrightarrow |P_{1/2}F=1\rangle$ following [37].

State detection is achieved using resonant light near 369 nm, which preferentially couples the state $|1\rangle$ to the excited $P$ state, resulting in a large probability of detecting scattered photons. These photons are detected using a pair of large-diameter lenses and a photomultiplier tube. State discrimination is conducted by photon counting followed by conversion to a probability that the Bloch vector lies at a particular location along a meridian of the Bloch sphere. This measurement is susceptible to ion loss in the ensemble and both laser amplitude and frequency drifts over long time scales, resulting in variable maximum and dark count rates over time. We therefore employ a normalization and Bayesian estimation procedure to improve measurement fidelity.

Dark-state normalization is achieved by cooling and optically pumping the ions to the $F=0$ state of the 12.6-GHz hyperfine manifold and then performing a measurement of photon counts, while bright-state normalization includes an additional $\pi$, gate implemented using microwaves before the photon count measurement. We have experimentally ascertained that for any angle of declination of the Bloch vector with respect to the $-z$ axis, $\theta$, photon counts over a repeated number of identical experiments are normally distributed about a mean value with standard deviation dominated by rapid laser frequency fluctuations with magnitude $\sim 1$ MHz.

We use Bayesian inference to statistically determine the qubits' $z$ projection given the number of scattered 369-nm photons we measure, denoted $P(\theta|c)$. We write

$$P(\theta|c) = \frac{P(c|\theta)P(\theta)}{P(c)} \quad (4.1)$$

$$= \frac{\sum_{\theta} \int_0^1 d\theta P(c|\theta)P(\theta)}{P(c)} \quad (4.2)$$

where in the second line we have incorporated the fact that $P(c)$ is dependent on our knowledge of the probability distribution function for $\theta$. We have experimentally verified that we may write the probability density function $P(c|\theta) = \exp\left[-\left(\frac{c^2}{2\sigma^2}\right)\right]$. Here, we have defined a Gaussian with center defined by linearly interpolating between the mean detected photon counts for the bright state $B$ and mean counts for the dark state $D$. The standard deviation of the Gaussian is defined by linearly interpolating between the standard deviations of the photon-count distributions for the bright state $\sigma_B$ and dark state $\sigma_D$. The quantities $B$, $D$, $\sigma_B$, and $\sigma_D$ are found by performing bright- and dark-state normalization before each iteration of the experiment of interest. $P(\theta)$ is initially assumed to be a uniform probability distribution, and is iteratively refined with subsequent experiments. We then calculate the mean and standard deviation and apply the transform $P(\theta) = \sin^2\left(\frac{\theta}{2}\right)$. Using this method, we can achieve measurement fidelity in excess of 98%.

A simpler method of calculating the approximate bright-state probability is to take a simple normalized average of the form $(E-D)/(B-D)$ where $B$ and $D$ are defined as before and $E$ is the mean detected photon count for the experiment of interest. This method agrees well with Bayesian estimation for states that are not near the poles of the Bloch sphere and provides a simpler and faster measurement method in cases where maximizing measurement fidelity near the poles is not required.

To produce our master oscillator signal we use an ultralow-phase-noise vector source referenced to a caesium clock and 10-MHz Wenzel cleanup oscillator for long-term stability and good short-term phase noise. The output of the signal generator is amplified using a low-phase-noise amplifier with maximum output of approximately +33 dBm. A commercially available, microwave horn-lens combination is used to produce a highly directional free-space linearly polarized microwave field (+25 dBi directional gain) which can be directed at the ions, approximately 150 mm from a 150-mm-diameter viewport on the UHV chamber.

Coherent rotations between the measurement basis states are driven using the magnetic field component of resonant microwave radiation. The Rabi rate for driven oscillations is linearly proportional to the microwave magnetic field amplitude, with rotations about an axis $\vec{r}$ lying on the $xy$ plane of the Bloch sphere and set by the phase of the microwaves as $\vec{r} = [\cos(\phi(t)), \sin(\phi(t)), 0]$. Rabi flopping experiments [Fig. 2(c)] demonstrate high-sensitivity coherent qubit rotations where we can achieve hundreds of flops before seeing appreciable decay. With $\sim +30$ dBm nominal microwave power (e.g., not accounting for cable losses) we achieve $\pi$ times as low as $\sim 15$ ms, but we typically operate near 50 ms. We have confirmed that in these experiments our measured Rabi flopping times are limited by small microwave field amplitude inhomogeneities over the ion ensemble caused by diffraction of the microwave beam at the aperture of the UHV chamber.

A standard technique for characterizing oscillator stability is Ramsey spectroscopy [44]. We prepare the ions in $|0\rangle$ and rotate to $|+\rangle$, using a $\pi/2$ pulse applied about $\hat{x}$, but slightly detuned from resonance by $+4$ Hz. After a free-evolution period, a second $\pi/2$ pulse will rotate the qubit to $|0\rangle$ or $|1\rangle$ depending on the phase accumulated between the master oscillator and the qubit. Scanning the evolution time $\tau$ reveals sinusoidal fringes due to the free evolution of the qubit relative to the control during the delay period. Instabilities of the phase over time cause the relative phase between the qubit and master oscillator to become randomized, thus reducing the visibility of Ramsey fringes.

An important advantage of this system is that the selected qubit transition is first order insensitive to magnetic field fluctuations. As a result, the intrinsic free-evolution coherence time of this hyperfine qubit has been measured to be at least 15 min [45]. A $T_2$ decay time of approximately 4 s, inferred from Ramsey experiments [Fig. 2(d)], demonstrates long-term coherence between the qubit and our LO, ultimately limited by phase stability of the LO (typically $-80$ dBc phase noise at 100 Hz offset from carrier). These experimental measurements reveal that this system therefore provides a "clean" baseline for quantitative tests of bath engineering.

B. Implementation of bath engineering by IQ modulation

The bath engineering technique described above provides a generic framework allowing noise to be generated for specific
Hamiltonians of interest. We must now demonstrate how such noise may be implemented using the kind of control hardware typically available for quantum control experiments: \( IQ \) modulation on the resonant carrier.

To model a desired control field in the presence of noise, we generate a microwave field of the form set out in Eqs. (2.2)–(2.4). In order to engineer the bath in our experimental system, we begin with a desired noise power-spectral density in either the amplitude or detuning quadrature (or both), assuming they are statistically independent. From this power spectrum, defined by the noise strength \( \alpha \), the exponent of the power-law scaling \( p \), the comb spacing \( \omega_0 \), and the high-frequency cutoff \( \omega_c \), we numerically generate time-domain vectors for \( \Omega(t) \) and \( \phi(t) \) using the relationships appearing in Sec. 2, and randomly selecting the phase \( \psi_j \) for each comb tooth in the Fourier decomposition. Thus, we may independently generate our control and noise modulation signals for the carrier amplitude and phase (see Fig. 3).

Independent and arbitrary control over these properties of the carrier may be achieved using \( IQ \) modulation [46]. \( I(t) \) and \( Q(t) \) are simply a polar-to-Cartesian coordinate transform of the familiar amplitude \( \Omega(t) \) and phase \( \phi(t) \) components of a modulated signal \( S(t) = \Omega(t) \sin[\omega_c t + \phi(t)] \) as

\[
S(t) = I(t) \sin(\omega_c t) - Q(t) \sin(\omega_c t - \pi/2),
\]

\[
I(t) = \Omega(t) \cos[\phi(t)], \quad Q(t) = \Omega(t) \sin[\phi(t)].
\]

The numerically generated noise and control modulation patterns are thus converted to the \( IQ \) basis and applied as a modulation pattern in time. While our method typically relies on a Fourier decomposition for the generation of the \( IQ \)-modulation patterns, arbitrary time-domain noise may be engineered, such as the influence of random telegraph noise in carrier frequency.

As mentioned above, our carrier frequency for the clock transition in \(^{171}\text{Yb}^+\) is 12.6 GHz, produced by a vector signal generator. The key feature of this unit is a digitally programmable baseband generator producing the modulation envelopes for \( I \) and \( Q \). The functions are defined sample-wise with 16-bit resolution in order to approximate a continuous function. In our system, care must be taken to ensure that discontinuities in the waveforms are avoided as the baseband generator employs an interpolation algorithm that can produce ringing in the applied modulation.

FIG. 2. (Color online) Experimental control system. (a) Simplified level structure of \(^{171}\text{Yb}^+\) ions with qubit at 12.6-GHz splitting highlighted. Solid arrows indicate excitation via UV detection laser, dotted arrows indicate spontaneous emission pathways. Repumping transitions to metastable \( D \) and \( F \) states not shown. (b) Microwave synthesis chain employed for \(^{171}\text{Yb}^+\) qubits. Digital programming of the vector signal generator (VSG) conducted via either GPIB or LAN. (c) Measured Rabi flopping at 12.6 GHz on the clock transition in the \(^{171}\text{Yb}^+\) ground state. In this measurement, we use Bayesian estimation to map raw measured photon counts to bright- or dark-state probability. (d) Free evolution measured via Ramsey interferometry and presented using raw photon counts for simplicity. Interrogating \( \pi/2 \) pulses applied with frequency detuning of \( \sim 4 \) Hz to yield interference fringes. After approximately 2 s of free evolution, the fringe frequency appears to shift abruptly and then become unstable. The overlaid damped oscillation assumes a Gaussian decay and a T2 of 4 s and matches the general decay envelope well. However, due to the appearance of statistically nonstationary dynamics during the experiment, fitting struggles to provide an accurate reproduction of the data. Nonetheless, the data clearly indicate coherence between the LO and qubits beyond approximately 3 s.

FIG. 3. (Color online) Schematic representation of process flow involved in experimental noise engineering. Independent waveforms for phase and amplitude are determined numerically, shifted to the \( IQ \) basis and sent to the dual digital-to-analogue converter (DAC) used for \( IQ \) modulation in our vector signal generator.

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C. Direct characterization of the microwave carrier

In order to quantitatively verify the noise engineering process, we begin by measuring the resultant phase noise on a 12.6-GHz carrier in the presence of bath engineering. Interpreting such data requires a brief quantitative analysis of the effect of amplitude and phase modulation as represented in the Fourier domain. In the case of amplitude modulation, a signal consisting of a single-frequency amplitude-modulated (AM) carrier can be expressed as

\[ S(t) = A_\mu + A_m \sin(\omega_0 t) \sin(\omega_m t) \]

\[ = A_\mu \sin(\omega_0 t) + A_m \cos(\delta t) - A_m \cos(\delta t), \]

where \( A_\mu \) and \( A_m \) are the amplitudes of the carrier and modulating sinusoid and \( \omega_0 \) and \( \omega_m \) are their frequencies, respectively. In the second line above we see the signal is represented as a weighted sum of the carrier frequencies as well as two symmetric sideband frequencies \( \delta = \omega_0 \pm \omega_m \) from the carrier. Referring back to Eq. (3.11), each comb tooth gives rise to a pair of sidebands with amplitude \( (\text{power}) \) proportional to \( \alpha F(j) \left| e^{i \Phi(j)} \right|^2 \). In this case, the power-law scalings of the comb teeth, \( p \), and the measured phase-noise power spectrum are identical.

The case of dephasing noise is slightly more complicated due to the effect of frequency or phase modulation as represented in the Fourier domain. Single-frequency phase modulation with amplitude \( \Phi_m \) at frequency \( \omega_m \) gives a signal

\[ S(t) = A_\mu \sin(\omega_0 t + \Phi_m \sin(\omega_m t)) \]

\[ = A_\mu \sum_{j=\infty} \sin(j \omega_0 t + \Phi_m \sin(\omega_m t)) \]

\[ \approx A_\mu \sin(\omega_0 t) + A_m \Phi_m \sin(\delta t) + A_m \Phi_m \sin(\delta t). \]

Such modulation produces an infinite comb of frequencies, centered around the carrier, spaced by \( \omega_m \), and weighted by Bessel functions [47]. In the last line above we have assumed small modulation depth allowing the infinite comb to be truncated beyond first order. As a result of this expression, the relationship between the power law of comb teeth in Eq. (3.7) and the expected form of the phase noise is \( p = (p - 2) \).

Phase-noise power spectra are presented in Figs. 4(a)–4(d) using units of dBc/Hz as a function of offset from the carrier, for different forms of bath engineering. These data provide a measure of the total power at a particular offset referenced to the carrier in a one-Hertz integration bandwidth. In all cases, we observe a strong increase in the measured phase noise over the (unmodulated) carrier noise floor up to a cutoff frequency corresponding to the programed \( \omega_m \). The form of decay in the phase-noise power law is well described using the expressions above, as indicated by guides to the eye superimposed on the measured data. Agreement is good for both amplitude and detuning noise. We also observe that as the noise strength (i.e., modulation depth) increases for dephasing noise, the first-order approximation above fails and the cutoff frequency is no
longer clearly visible in these plots due to the infinite comb of sidebands.

D. Qubits in a noisy bath

We quantitatively demonstrate our bath engineering techniques by studying the effect of engineered dephasing noise on the free evolution of our trapped-ion qubits. We produce time-domain dephasing noise using a discrete comb with fundamental frequency \( \omega_0 = 2\pi \times 4 \) Hz, and a cutoff \( \omega_c = 2\pi \times 3 \) kHz. Selecting \( F(j) = j^{-1} \) yields a white-dephasing-noise power-spectral density.

In our experiments, we perform Ramsey spectroscopy in the presence of engineered noise. We observe the decay time constant of fringe visibility is significantly reduced in the presence of the engineered bath, as expected. A representative Ramsey experiment is presented in the inset of Fig. 4(e) showing the fringe visibility decays over a time scale of order milliseconds in the presence of the engineered bath. Since Ramsey spectroscopy measures the relative coherence between two oscillators (the LO and the qubit), engineered dephasing in the LO results in net decoherence even during free-evolution periods.

The scaling of the measured coherence time with noise strength is a key validation of our bath engineering techniques. We write the ensemble-averaged coherence for free evolution in the presence of dephasing noise as \( W(t) = \exp(-\chi(t)) \) [48,49] where \( \chi(t) = \frac{2}{\pi} \int_{\omega_c}^{\infty} \frac{S_{\beta}(\omega) \sin(\omega t/2)}{(\omega \tau)^2} \) \( d\omega \) [21]. Incorporating the relevant form of \( S_{\beta}(\omega) \) gives

\[
\chi(t) = 2\alpha^2 \omega_0^2 \sum_{j=1}^{750} \frac{\sin^2(j\omega_0 t/2)}{(j\omega_0)^2},
\]

where the upper limit on the sum is determined from the specifics of the comb tooth spacing and noise cutoff frequency. The expected decay envelope resulting from the integral above and for our value of \( \omega_0 \) is a simple exponential, although slight modification yields more complex functional forms (see Appendix C). As a result, we expect a quadratic scaling of the decay time constant with \( \alpha \).

We study the scaling of the \( 1/e \) coherence time \( T_\chi \) as a function of the noise strength, parametrized by \( \alpha \). Ramsey fringes are recorded for each value of \( \alpha \) and a fit to a sinusoid with a simple exponential decay envelope is performed in order to extract \( T_\chi \). These data are plotted as the decay rate \( T_\chi^{-1} \) of the qubit coherence as a function of \( \alpha \) in Fig. 4(e). The decay rate is observed to scale as \( T_\chi^{-1} \propto \alpha^2 \), as expected, with the overall decay time scales determined by the specifics of the noise power-spectral density.

Similarly, we study driven evolution such as that presented in Fig. 2(c), but now in the presence of engineered amplitude noise [Figs. 4(f)–4(i)]. Increasing the strength of the noise results in a Gaussian decay envelope for the Rabi flopping data with decreasing decay constants. The evolution of the measured decay constant does not take a convenient analytic form with noise strength and so we perform numerical integration of the Schrödinger equation considering a driving field with the same noise characteristics. The data show good agreement with the numerical calculations qualitatively and quantitatively.

Other experiments incorporating dephasing noise during driven evolution and/or universal noise also reveal behavior in quantitative agreement with the formulation provided above, but form the subject of separate papers. Overall, these measurements validate the efficacy of our approach in generating a quantitatively useful noise bath in a real quantum system.

V. CONCLUSION

In this paper, we have presented a detailed technical prescription for the quantitative engineering of unitary baths for studies of quantum control. We produce a discrete comb of noise frequencies possessing an overall scaling chosen to reproduce a noise power spectrum of interest in either the dephasing or amplitude-damping quadrature. We show how this technique lends itself to simple numerical construction of complex time-dependent noise processes using common I-Q-modulated carriers for single-qubit control. We validate our technique through both examination of the modulation form on a vector signal analyzer and through application of engineered dephasing noise to the free evolution of trapped \( ^{171}\text{Yb}^+ \) ions. Our measurements demonstrate that the coherent lifetime of the qubits probed by a 12.6-GHz carrier incorporating engineered noise scales as expected based on a simple physical model.

The technique we present is applicable to a wide variety of experimental systems employing carrier signals in the rf or microwave. It is particularly useful in trying to understand the spectral sensitivity of various quantum control protocols such as dynamical decoupling and dynamically corrected gates. For instance, our group has utilized this technique to quantitatively validate the error-suppressing properties of novel classes of modulated error-suppressing gates, as will be described in future papers. The incorporation of engineered noise in such experiments is vital to help elucidate the bounds and performance scaling of such protocols in regimes where the measured errors (the signal of interest) are in general not sufficiently large to exceed intrinsic state preparation and measurement errors. It is also possible to combine this kind of unitary noise engineering with dissipation [50–53], for instance, through leakage of off-resonant lasers or otherwise inducing spontaneous emission properties, or to expand the general technique to multilevel manifolds [8]. We hope that our general technique will prove useful to the quantum control and quantum information communities as they push towards ultrahigh-fidelity gate operations.

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are those of the authors and should not be construed as representing the official views or policies of IARPA, the ODNI, or the US Government.

APPENDIX A: DERIVATION OF THE SYSTEM HAMILTONIAN

The system considered in this paper consists of a qubit with transition (angular) frequency $\omega_0$, driven by a local oscillator with magnetic field component aligned with $\delta_0$ taking the form

$$B(t) = \Omega(t) \cos(\omega_0 t + \phi(t)) \hat{z},$$

(A1)

$$\Omega(t) = \Omega_c(t) + \Omega_y(t),$$

(A2)

$$\phi(t) = \phi_c(t) + \phi_y(t)$$

(A3)

with $\omega_0$ the carrier frequency. In this formulation, the time dependence of the phase $\phi(t)$ and amplitude $\Omega(t)$ has been formally partitioned into components denoted by the subscripts $c$ and $y$, capturing the desired control and noisy interactions, respectively. Using the dipole approximation, the system Hamiltonian ($\hbar = 1$) in the laboratory frame is

$$H_S = \frac{\omega_0}{2} \hat{\sigma}_z + \Omega(t) \cos(\omega_0 t + \phi(t)) \hat{\sigma}_z,$$

(A4)

The first term corresponds to the Hamiltonian of the qubit under free evolution, and the second term corresponds to the qubit-field interaction. Moving to the interaction picture corotating with the carrier frequency and making the rotating-wave approximation, the dynamics are described by the Hamiltonian

$$H_s^{(\omega_0)} = \left( \frac{\Delta}{2} \right) \hat{\sigma}_z + \frac{1}{4} \Omega(t) e^{-i \phi(t)} \hat{\sigma}_+ + e^{i \phi(t)} \hat{\sigma}_-,$$

(A5)

where $\Delta = \omega_0 - \omega_0$ is the carrier detuning from the transition frequency, and we define the usual operators $\hat{\sigma}_\pm = \hat{\sigma}_x \pm i \hat{\sigma}_y$. Setting $\Delta = \phi_0(t) = 0$, Eq. (A5) reduces to $H_s^{(\omega_0)} = \frac{1}{2} \Omega(t) \cos(\phi(t)) \hat{\sigma}_z + \sin[\phi(t)] \hat{\sigma}_x$, so the resonant carrier field drives coherent Rabi flopping between the qubit states $|1\rangle$ and $|0\rangle$. The instantaneous Rabi rate in this case is proportional to $\Omega(t)$ and rotations, generated by the spin operator $\hat{\sigma}_{xy}(t)$, are driven about the axis $\hat{r} = [\cos \phi_c(t), \sin \phi_c(t), 0]$ in the $xy$ plane of the Bloch sphere. For instance, a noise-free $\pi$ pulse about the $x$ axis would have $\Omega_x, \phi_x, \phi_c = 0$, and $\Omega_c(t) = \Omega$ for $t \in [0, \tau_x]$, with $\tau_x = \pi/\Omega$. The noise component $\phi_y(t)$ of the engineered phase $\phi(t)$, in the exponentials of Eq. (A5), may be mapped to rotations about $\hat{\sigma}_z$ if we move to a second interaction picture defined by

$$H_s^{(\omega_0, \phi_y)} := \hat{U}_{\delta_0} H_s^{(\omega_0)} \hat{U}_{\delta_0} - H_{\phi_y},$$

(A6)

where $\hat{U}_{\delta_0} := \exp[\frac{\delta_0(t)}{2} \hat{\sigma}_z]$ is the evolution operator under the the engineered dephasing Hamiltonian $H_{\phi_y} := \frac{1}{2} \phi_y(t) \hat{\sigma}_z$. Setting the carrier detuning $\Delta = 0$, it is then straightforward to show

$$H_s^{(\omega_0, \phi_y)} = -\phi_y(t) \frac{1}{2} \hat{\sigma}_z + \frac{1}{2} \Omega(t) \cos[\phi_c(t)] \hat{\sigma}_z + \sin[\phi_c(t)] \hat{\sigma}_x + e^{-i \omega_y t} \hat{\sigma}_- + e^{i \omega_y t} \hat{\sigma}_+.$$  

(A7)

APPENDIX B: DERIVATION OF NOISE POWER-SPECTRAL DENSITIES

Let $h(t)$ be any time-dependent function. We use nonunitary angular frequency notation consistent with the usage in Ref. [50] to define a Fourier transform pair

$$H(\omega) = \mathcal{F}[h(t)] = \int_{-\infty}^{\infty} h(t) e^{-i \omega t} dt,$$  

(B1)

$$h(t) = \mathcal{F}^{-1}[H(\omega)] = \frac{1}{2\pi} \int_{-\infty}^{\infty} H(\omega) e^{i \omega t} d\omega.$$  

(B2)

In this case, a time-domain signal $\beta(t)$ is related to its PSD $S_\beta(\omega)$ by the Wiener-Khintchine theorem [43] which takes the form

$$\langle \beta(t_1) \beta(t_2) \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} S_\beta(\omega) e^{i \omega (t_1 - t_2)} d\omega.$$  

(B3)

In this paper, we assume all noise processes are wide-sense stationary in which case the two-point correlation function $\langle \beta(t_1) \beta(t_2) \rangle$ depends only on the relative difference $\tau = t_2 - t_1$ between $t_1$ and $t_2$ and reduces to the autocorrelation function $C_\beta(\tau) := \langle \beta(t) \beta(t + \tau) \rangle$. The angle brackets now denote averaging over all times $t_1$ with respect to which the relative lag $\tau$ is defined. Consequently, $C_\beta(\tau) = \frac{1}{2\pi} \int_{-\infty}^{\infty} S_\beta(\omega) e^{i \omega \tau} d\omega$, or using Eqs. (B1) and (B2),

$$S_\beta(\omega) = \mathcal{F}[C_\beta(\tau)] = \int_{-\infty}^{\infty} \langle \beta(t) \beta(t + \tau) \rangle e^{-i \omega \tau} d\tau.$$  

(B4)

1. Dephasing-noise PSD

We require an expression for the autocorrelation function of $\beta(t)$, the dephasing-noise field, in order to derive the corresponding PSD $S_\beta(\omega)$ given by Eq. (B4). Using Eq. (3.5), it is straightforward to show

$$\langle \beta(t + \tau) \beta(t) \rangle = \frac{\alpha^2 \alpha_0^2}{4} \sum_{j,j'} \int_j j' F(j) F(j') e^{i \omega_0 \tau} e^{i \omega_{j+j'} \tau} e^{i \omega_j \Psi_{j+j'}},$$

(B5)

Or, averaging over $\tau$,

$$\langle \beta(t + \tau) \beta(t) \rangle = \frac{\alpha^2 \alpha_0^2}{4} \sum_{j,j'=1} \int_j j' F(j) F(j') e^{i \omega_0 \tau} e^{i \omega_{j+j'} \tau} e^{i \omega_j \Psi_{j+j'}},$$

(B5)

Since $\omega_{j+j'}$ are always positive, we know $\alpha_0 \alpha_j$ is always positive. Consequently, the term $e^{i \omega_{j+j'} \tau}$ is always an oscillating term with nonzero frequency $\pm (\omega_j + \omega_j')$ and
average over $t$ yields
\[ \langle e^{\pm i(\omega_j + \omega_{j'})t} \rangle_t = 0. \tag{B6} \]
Similarly, when $\pm (\omega_j - \omega_{j'})$ is nonzero (i.e., when $\omega_j \neq \omega_{j'} \iff j \neq j'$), we have
\[ \langle e^{\pm i(\omega_j - \omega_{j'})t} \rangle_t = 0, \quad j \neq j'. \tag{B7} \]
However, when $\omega_j = \omega_{j'}$ (which occurs when $j = j'$)
\[ \langle e^{\pm i(\omega_j - \omega_{j'})t} \rangle_t = 1, \quad j = j'. \tag{B8} \]
or more concisely
\[ \langle e^{\pm i(\omega_j - \omega_{j'})t} \rangle_t = \delta_{jj'}, \tag{B9} \]
where $\delta_{jj'}$ is the Kronecker delta. Thus, the autocorrelation function for $\beta_j(t)$ takes the form
\[
\langle \beta_j(t + \tau) \beta_j(t) \rangle_t = \frac{\alpha^2 \omega_0^2}{4} \sum_{j,j'=1}^J j^2 F(j)^2 \left[ e^{2i\omega_0 t} + e^{-2i\omega_0 t} \right]
\times \left[ e^{i(\phi_j - \phi_{j'})} \delta_{jj'} + e^{-i(\phi_j - \phi_{j'})} \delta_{j'j} \right] \tag{B10} \]
\[ = \frac{\alpha^2 \omega_0^2}{2} \sum_{j=1}^J j F(j)^2 \cos(\omega_j \tau). \tag{B11} \]
Substituting this into Eq. (B4) yields
\[
S_\gamma(\omega) = \int_{-\infty}^{\infty} \langle \beta_j(t) \beta_j(t + \tau) \rangle_t e^{-i\omega \tau} d\tau
\]
\[ = \frac{\alpha^2 \omega_0^2}{2} \sum_{j=1}^J j F(j)^2 \cos(\omega_j \tau) \tag{B12} \]
\[ = \frac{\alpha^2 \omega_0^2}{2} \sum_{j=1}^J j F(j)^2 \mathcal{F}[\cos(\omega_j \tau)]. \tag{B13} \]
Using the result from Fourier analysis that
\[
\mathcal{F}[\cos(\omega' \tau)] = \int_{-\infty}^{\infty} \cos(\omega' \tau)e^{-i\omega \tau} d\tau
\]
\[ = \pi [\delta(\omega - \omega') + \delta(\omega + \omega')]. \tag{B14} \]
we therefore obtain our result
\[ S_\gamma(\omega) = \frac{\alpha^2 \omega_0^2}{2} \sum_{j=1}^J j F(j)^2 \left[ \pi \delta(\omega - \omega_j) + \delta(\omega + \omega_j) \right]. \tag{B15} \]

2. Amplitude-noise PSD

We require an expression for the autocorrelation function of $\beta_j(t)$, the amplitude-noise field, in order to derive the corresponding PSD $S_\alpha(\omega)$ given by Eq. (B4). Using Eq. (3.11), and following the same procedure used in the above section, it is straightforward to show
\[
\langle \beta_j(t + \tau) \beta_j(t) \rangle_t = \frac{\alpha^2}{2} \sum_{j=1}^J j F(j)^2 \cos(\omega_j \tau). \tag{B16} \]
Substituting this into Eq. (B4) and using Eq. (B16), we therefore obtain the result
\[ S_\alpha(\omega) = \frac{\alpha^2}{2} \sum_{j=1}^J j F(j)^2 \mathcal{F}[\cos(\omega_j \tau)] \tag{B17} \]
\[ = \frac{\pi \alpha^2}{2} \sum_{j=1}^J j F(j)^2 \delta(\omega - \omega_j) + \delta(\omega + \omega_j). \tag{B18} \]

APPENDIX C: DEPENDENCE OF $\chi$ ON $\tau$ FOR FID

In the case of a pure white-noise-detuning PSD it is relatively simple to calculate an exact form for $\chi(\tau)$. Starting with $\chi(\tau) = \frac{1}{2} \int_{-\infty}^{\infty} \frac{\sin^2(\omega/2) d\omega}{\omega^2}$ and incorporating

![Graphs showing the dependence of $\chi$ on $\tau$ for various choices of $\omega_0$.](image-url)
producing a coherence integral
\[
\chi(\tau) = 2\alpha^2 \sum_{j=1}^{750} \frac{\sin^2(j\omega_0\tau/2)}{(j\omega_0)^2},
\] (C2)

where \(\omega_0 = 4\) Hz. In such circumstances, we rely on numerical calculations to determine the behavior \(\chi(\tau)\) over the time interval relevant to the Ramsey spectroscopy experiments in Fig. 5(a). For our choice of \(\omega_0\) we find good approximation of the integral to a linear function of \(\tau\), suggesting the use of a simple exponential fit to Ramsey decay in free-induction decay (FID) experiments with engineered noise. However, we observe that modifying the fundamental frequency of the power spectrum changes the dependence of \(\chi(\tau)\) within the same evolution time interval, requiring careful attention to the noise model in use when performing quantitative studies of bath engineering.

Appendix C

arXiv pre-print
Improving frequency standard performance by optimized measurement feedback

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We demonstrate a new approach to precision frequency standard characterization and stabilization, providing performance enhancements in the presence of non-Markovian noise in the local oscillator with “software-only” modifications. We develop a theoretical framework casting various measures for frequency standard variance in terms of frequency-domain transfer functions, incorporating the effects of feedback stabilization via a chain of Ramsey measurements. Using this framework we introduce a novel optimized hybrid feedforward measurement protocol which employs results from multiple measurements and transfer-function-based calculations of measurement covariance given the local oscillator power spectrum. This approach exploits statistical correlations in the local oscillator frequency noise to provide high-accuracy corrections in the presence of uncompensated dead time in the measurement cycle or oscillator-frequency evolution during the Ramsey measurement period itself. We present numerical simulations of oscillator performance under competing feedback schemes and demonstrate benefits in both correction accuracy and long-term oscillator stability using hybrid feedforward.

High-performance frequency standards play a major role in technological applications such as network synchronization and GPS [1] as well as many fields of physical inquiry, including radioastronomy (very-long-baseline interferometry) [2], tests of general relativity [3], and particle physics [4]. Atomic clocks exploiting the stability of Cs [5–8] or other atomic references [9–13] are known as the most precise timekeeping devices available, but constant performance gains are sought for technical and scientific applications.

A major limit to the performance of passive frequency standards comes from the quality of the local oscillator (LO) used to interrogate the atomic transition. The LO frequency evolves randomly in time due to intrinsic instabilities from the underlying hardware [10, 11], leading to deviations of the LO frequency from that of the stable atomic reference. These instabilities are partially compensated through use of a feedback protocol designed to transfer the stability of the reference to the LO, but their effects cannot be mitigated completely. LO fluctuations ultimately produce instabilities in the locked local oscillator (LLO) due to both uncompensated noise during initialization and readout stages of the measurement cycle (dead time), as well as phenomena such as aliasing of noise at harmonics of the feedback-loop period, known as the Dick effect [14–16]. Accordingly, significant research focus in the frequency standards community has been placed on improving LO performance, using e.g. ultra-low-phase-noise cryogenic sapphire oscillators or similar [17, 18], with concomitant increases in hardware infrastructure requirements and complexity.

In this Letter we demonstrate a method by which both the accuracy and stability of passive frequency standards can be improved without the need for hardware modification. We present a new theoretical framework capturing the effects of LO noise and feedback protocols in the frequency domain in order to calculate the expected correlations between multiple sequential measurements. Thus, given statistical knowledge of the LO noise characteristics, we are able to produce a new form of hybrid feedforward stabilization incorporating the results of an arbitrary number of past measurements with variable duration to calculate an improved correction to the LO. In cases where dead time is significant and there is substantial uncompensated LO evolution, we show that this approach allows corrections with improved accuracy to be applied to the frequency standard. Numerical simulations also demonstrate that long-term stability of the LLO is improved through a moving-average correction scheme, where corrections are made based on weighting values determined analytically in the same hybrid feedforward approach. The method described here is a technology-independent software-oriented approach to improving the performance of frequency standards.

Ramsey spectroscopy provides a means to determine the average fractional frequency offset over a period, $T_N$; this information is used to determine the correction to be applied in the standard LO feedback loop (Fig. 1a). We represent the fractional frequency offset of an LO relative to an ontologically perfect (atomic) reference $y(t) = (\nu(t) - \nu_0)/\nu_0$, where $\nu_0$ is the reference frequency and $\nu(t)$ is the LO frequency. A Ramsey measurement performed over the $k$th time interval $[t_{k}\downarrow, t_{k}\uparrow]$, with duration $T_{N}^{(k)} \equiv t_{k}\uparrow - t_{k}\downarrow$, is characterized by a sensitivity function $g(t) \in [0, 1]$, capturing the extent to which LO fluctuations at some instant $t$ contribute to the measured outcome for that interval [19], yielding measurement outcome $\hat{y}_{k} = \frac{1}{T_{N}^{(k)}} \int_{t_{k}\downarrow}^{t_{k}\uparrow} y(t) \nu(t) \nu(t) dt$. In the case of a square sensitivity function over the Ramsey period, the form of

$$
\int_{t_{k}\downarrow}^{t_{k}\uparrow} y(t) \nu(t) \nu(t) dt = \frac{1}{4} (t_{k}\uparrow - t_{k}\downarrow)^2.
$$

$$
\int_{t_{k}\downarrow}^{t_{k}\uparrow} y(t) \nu(t) \nu(t) dt = \frac{1}{4} (t_{k}\uparrow - t_{k}\downarrow)^2.
$$

$$
\int_{t_{k}\downarrow}^{t_{k}\uparrow} y(t) \nu(t) \nu(t) dt = \frac{1}{4} (t_{k}\uparrow - t_{k}\downarrow)^2.
$$


\[ g(t) \]

The performance of the frequency standard is statistically characterized, for instance, by the time-domain sample variance \( \sigma_y^2[N] = \frac{1}{N} \sum_{k=1}^{N} (\bar{y}_k - \bar{t})^2 \) for \( N \) sequential finite-duration measurements \( \{\bar{y}_k\} \). This metric captures the evolution of LO frequency as a function of time. Similarly we may define the true variance of \( \bar{y}_k, \sigma_y^2(k) = E[\bar{y}_k^2] \), equal to the expected value of \( \bar{y}_k^2 \), since \( g(t) \) is assumed to be a zero-mean process. The true variance captures the spread of measurement outcomes due to different noise realizations in a single timestep. Applying feedback corrections sequentially after measurements is able to effectively reduce \( g(t) \) over many cycles, improving long-term stability; whether the sample or the true variance is used, larger variance corresponds to a frequency standard with greater fractional uncertainty (worse performance).

Despite the power of feedback stabilization, evolution of \( g(t) \) during a measurement period, \( T_c \), can cause frequency deviations that are uncompensated in the feedback loop, limiting the accuracy of the corrections and increasing the statistical variance of the locked frequency standard. These effects are exacerbated in circumstances where dead time, \( T_D \), is substantial, due, for instance, to the need to reinitialize the reference between measurements (Fig. 1b). We require an efficient theoretical framework in which to capture these effects, and hence transition to the frequency domain, making use of the power spectral density of the LO, \( S_y(\omega) \), in order to characterize average performance over a hypothetical statistical ensemble. In this description residual LLO instability persists because the feedback is insensitive to LO noise at high frequencies relative to the inverse measurement period. Additional instability due to the Dick effect comes from aliasing of noise at harmonics of the loop bandwidth.

We may calculate the effects of measurement, dead-time, and the feedback protocol itself on frequency standard performance in the frequency domain as follows. A normalized, time-reversed sensitivity function \( \bar{g}(t_m^c - t) = g(t - t_m^c)/T_{f(k)}^c \), where \( g(t) \) is assumed to be time-reversal symmetric about \( t_m^c \), the midpoint of \([t_m^c, t_m^c] \), we can express, for instance, the true variance as a convolution \( \sigma_y^2(k) = E\left( \int_{-\infty}^{\infty} g(t)\bar{g}(t_m^c - t)dt \right)^2 \). Expanding this expression and using the Wiener-Khinchin theorem gives the true variance of measurement outcomes as an overlap integral \( \sigma_y^2(k) = \frac{1}{\pi} \int_0^{\infty} S_y(\omega) |G_k(\omega)|^2 d\omega \), with \( G_k(\omega) \equiv \int_{-\infty}^{\infty} \bar{g}(t_m^c - t)e^{i\omega t}dt \). Here \( |G_k(\omega)|^2 \) is called the transfer function for the kth sample. For measurements performed using Ramsey interrogation with \( \pi/2 \) pulses of negligible duration and zero dead time, the transfer function has a sinc-squared analytic form \( |G_k(\omega)|^2 = (\sin(\omega T_{f(k)}^c/2))^2/|\omega T_{f(k)}^c/2|^2 \).

We thus see that this approach allows expression of time-domain LO variances as overlap integrals between \( S_y(\omega) \) and the transfer function, \( |G(\omega)|^2 \), capturing the effects of the measurement and feedback protocols. Through this formalism we may calculate analytic expressions for measures such as the true variance, sample variance and Allan variance for either free-running LOs or LLOs undergoing feedback stabilization, and it permits incorporation of arbitrary measurement protocols (e.g. arbitrary and dynamic Ramsey periods and dead times) (see Supplementary Material).

This approach is powerful because it may also be employed to craft new measurement feedback protocols designed to improve the performance of the LLO. In particular we aim to mitigate the deleterious effect of dead time on LLO accuracy and stability by combining information from multiple measurements with statistical information about LO noise, \( S_y(\omega) \). Our key insight is that the non-Markovianity of dominant noise processes in typical LOs - captured through the low-frequency bias in \( S_y(\omega) - \)

![FIG. 1. (a) Simulated traces for a noisy LO, unlocked (red) and locked with traditional feedback (black), with correction period \( T_c \). The dotted horizontal bars indicate the measurement outcomes (samples) over each cycle, which are applied as correction at the end of the cycle (assuming zero dead time). The arrows on the far right schematically indicate how locking reduces the variance of \( g(t) \) though it does not eliminate it. (b) Schematic timing diagram of a standard feedback protocol with Ramsey measurement time, \( T_R \) and dead time \( T_D \), where \( T_D + T_R = T_c \). (c) Schematic diagram of hybrid feedforward with an example protocol with \( n = 3 \), with the option of non-uniform duration measurements instead of the uniform measurements illustrated here. Corrections \( C_k^{(n=3)} \) are applied in either non-overlapping blocks of three measurements or as a moving average (depicted here). In the latter case, the covariance matrix must be recalculated to correctly account for any variations in measurement duration. Dashed red arrows indicate the first corrections performed without full calculation of the covariance matrix. This effect vanishes for \( k > n \).](image-url)
implies the presence of temporal correlations in $y(t)$ that may be exploited to improve feedback stabilization.

The formal basis of our approach is a frequency-domain measure of correlation between time-separated measurements, using transfer functions derived here. In summary, we calculate a covariance matrix in the frequency domain via transfer functions to capture the relative correlations between sequential measurement outcomes of an LLO, and use this matrix to derive a linear predictor of the noise at the moment of correction. This predictor provides a correction with higher accuracy than that derived from a single measurement for experimentally-relevant noise spectra, allowing us to improve the performance of the LLO. Since the predictor is found using information from previous measurements (feedback) and a priori statistical knowledge of the LO noise (feedforward), we call the scheme hybrid feedforward. Effectively, we are able to predict the evolution of $y(t)$ by exploiting correlations captured statistically in $S_y(\omega)$, allowing feedback stabilization with increased accuracy and reduced sensitivity to dead time.

In hybrid feedforward, results from a set of $n$ past measurements are linearly combined with weighting coefficients $c_k$ optimized such that the $k$th correction, $C_k$, provides maximum correlation of $y(t_k)$ to samples $y_{k-l}$ (Fig. 1c). Assuming that the LO noise is Gaussian, the optimal least minimum mean squares correction with increased accuracy under hybrid feedforward is given by $C_k = c_k \cdot \bar{y}_k$, the dot product of a set of correction coefficients $c_k$ derived from knowledge of $S_y(\omega)$ and a set of $n$ past measured samples, $\bar{y}_k = \{\bar{y}_{k-1}, \cdots, \bar{y}_{k-n}\}$. We define an $(n+1) \times (n+1)$ covariance matrix where the $(n+1)$th term represents an ideal zero-duration sample at $t_k$ and in the second line we write the covariance matrix in block form:

$$
\Sigma_k = \begin{bmatrix}
\sigma(y_{k-1}, y_{k-1}) & \cdots & \sigma(y_{k-1}, y(t_k)) \\
\sigma(y_{k-2}, y_{k-1}) & \cdots & \sigma(y_{k-2}, y(t_k)) \\
\vdots & \cdots & \vdots \\
\sigma(y(t_k), y(t_k)) & \cdots & \sigma(y(t_k), y(t_k))
\end{bmatrix} 
$$

(1)

$$
\equiv \begin{bmatrix}
M_k \\
F_k \bar{y}_k
\end{bmatrix} = \begin{bmatrix}
\sigma(y(t_k), y(t_k))
\end{bmatrix}. 
$$

(2)

The MMSE optimality condition is then fulfilled for

$$
c_k = \frac{F_k}{\sqrt{F_k^T M_k F_k}} \int_0^\infty S_y(\omega) d\omega 
$$

(3)

where $w_k$ is an overall correction gain.

The covariance matrix elements are calculated as spectral overlap $\sigma(y_k, y_l) = \frac{1}{2\pi} \int_0^\infty S_y(\omega)G_{\omega,l}^2(\omega) d\omega$ using a pair covariance transfer function

$$
G_{\omega,l}^2(\omega) = \left| \frac{\omega^2 T_R^2 - \omega^2 l_R^2}{\omega^2 T_R^2} \right| \left( \cos(\omega(t_k - t_l)) + \cos(\omega(t_k - t_l)) \right)
$$

(4)

in the case of arbitrary-length Ramsey interrogations over the intervals $[t_k^i, t_k^f]$ (see Supplementary Material). This is a generalization of the transfer function previously derived for the special case of periodic, equal-duration Ramsey interrogations [19, 20], and allows effective estimation of $y(t)$ for any $t$ and for any set of measured samples $\bar{y}_k$.

In the practical setting of a frequency standard experiment, we wish to improve both the accuracy of each correction, by maximising the correlation between $C_k$ and $y(t_k)$, and the long-term stability of the LLO output, captured by the metrics of frequency variance, sample variance, and Allan variance. In order to test the general performance of hybrid feedforward in different regimes we perform numerical simulations of noisy LOs with user-defined statistical properties, characterized by $S_y(\omega)$. We produce a fixed number of LO realizations in the time domain and then use these to calculate measures such as the sample variance over a sequence of “measurement” outcomes with user-defined Ramsey measurement times, dead times, and the like. In these calculations we may assume that the LO is free running, experiencing standard feedback, or employing hybrid feedforward, and then take an ensemble average over LO noise realizations. Our calculations include various noise power spectra, with tunable high-frequency cutoffs, including common ‘flicker frequency’ ($S_y(\omega) \propto 1/\omega$), and ‘random walk frequency’ ($S_y(\omega) \propto 1/\omega^2$) noise, as appropriate for experiments incorporating realistic LOs.

We begin by studying the improvement in correction accuracy associated with a single correction cycle, defined as the extent to which a correction brings $y(t)$ towards $y(t_k)$ at the instant of correction, and then calculate a metric for accuracy as the inverse of frequency variance at $t_k$ relative to the free-running LO, $A_k \equiv \frac{\int_0^\infty S_y(\omega)^{-1} d\omega}{\int_0^\infty S_y(\omega) d\omega}$. Closed form analytic expressions for correction accuracy may be calculated in terms of elements of the covariance matrix (see Supplementary Material).

Tunability in the hybrid feedforward protocol comes from the number of measurements to be combined, $n$, in determining $\{C_k\}$ as well as the selected Ramsey periods, permitting an operator to sample different parts of $S_y(\omega)$. As an example, we fix our predictor to consider $n = 2$ sequential measurements and permit the Ramsey durations to be varied as optimization parameters. A Nelder-Mead simplex optimization over the measurement durations finds that a hybrid feedforward protocol consisting of a long measurement period followed by a short period maximizes feedback accuracy (Fig. 2a). This structure ensures that low-frequency components of $S_y(\omega)$ are sampled but the measurement sampling the highest frequency noise contributions are maximally correlated with $y(t_k)$. With $S_y(\omega) \propto 1/\omega$ and $S_y(\omega) \propto 1/\omega^2$ we observe increased accuracy under hybrid feedforward while the rapid fluctuations in $y(t)$ arising from a white power spectrum mitigate the benefits of hybrid feedforward, as expected. In the parameter ranges we have studied numerically we find that correction accuracy is max-
imized for \( n = 2 \) to 3, with diminishing performance for larger \( n \).

In all slaved frequency standards we rely on repeated measurements and corrections to provide long-term stability, a measure of how the output frequency of the LLO deviates from its mean value over time. We study this by calculating the sample variance of a time-sequence of measurement outcomes averaged over an ensemble of noise realizations, \( \langle \sigma_y^2 (N) \rangle \). A “moving average” style of hybrid feedforward provides improved long-term stability, as the correction \( C_k \) will depend on the set of measurement outcomes \( \{ y_k, y_{k-1}, \ldots, y_{k-n} \} \), among which previous corrections have been interleaved, as illustrated in Fig. 1c.

In Fig. 2b we demonstrate the resulting normalized improvement in \( \langle \sigma_y^2 (N) \rangle \) up to \( N = 100 \) measurements, calculated using feedback and hybrid feedforward with \( n = 2 \), and assuming uniform \( T_R \). We observe clear improvement (reduction) in \( \langle \sigma_y^2 (N) \rangle \) through the hybrid feedforward approach, with benefits of order \( 5 - 25\% \) of \( \langle \sigma_y^2 (N) \rangle \) relative performance improvement over standard measurement feedback. We present data for different functional forms of \( S_\nu (\omega) \), including low-frequency dominated flicker noise \( \langle 1/\omega \rangle \), and power spectra \( \langle 1/\omega^{1/2} \rangle \) with more significant noise near \( T_c^{-1} \). The benefits of our approach are most significant in the long term when high-frequency noise reduces the efficacy of standard feedback.

The improvement provided by hybrid feedforward is most marked for low duty factor \( d \), defined as the ratio of the interrogation time to total cycle time: \( d \equiv T_R/T_c \). As \( d \to 1 \) we observe that the feedback and hybrid feedforward approaches converge, as standard feedback corrections become most effective when dead time is shortest. However as the dead time increases, feedback efficacy diminishes until \( \langle \sigma_y^2 (N) \rangle \) for the feedback-locked LO approaches that for the free-running LO (value unity in Fig. 2c). In this limit the utility of the measurement-feedback diminishes as the LO noise evolves substantially during the dead time, but even here knowledge of correlations in the noise allows hybrid feedforward to provide significant gains in stability. In Fig. 2c we demonstrate that in the presence of a typical \( 1/\omega \) power spectrum, the presence of noise spurs near \( \omega/2\pi \approx T_c^{-1} \) results in certain regimes where standard feedback makes long-term stability worse, while feedforward provides useful stabilization. Exact performance depends sensitively on the form and magnitude of \( S_\nu (\omega) \), but results demonstrate that systems with high-frequency noise content around \( \omega/2\pi \approx T_c^{-1} \) benefit significantly from hybrid feedforward.

In this work we have relied on measures of frequency stability such as the true variance and sample variance, rather than the more commonly employed Allan variance, in line with recent experiments [21]. This selection has been deliberate as the form of the Allan variance specifically masks the effect of LO noise components with long correlation times. In fact the Allan variance, taking the form \( A^2 \sigma_y^2 (\tau) \) is employed by the community in part because it does not diverge at long integration times \( \tau \) due to LO drifts, as would the sample or true variance [19, 20, 22, 23]. In numerical calculations we do not observe significant improvements in \( A^2 \sigma_y^2 (\tau) \) using hybrid feedforward. However we note that this is only an artefact of characterization - the LLO is actually experiencing smaller average deviations relative to the stable frequency reference when using hybrid feedforward.

In summary, we have presented a set of analytical tools describing LLO performance in the frequency domain for
arbitrary measurement times, durations, and duty cycles. We have employed these generalized transfer functions to develop a new software approach to LO feedback stabilization in enslaved passive frequency standards. This technique leverages a series of past measurements and statistical knowledge of the noise to improve the accuracy of feedback corrections and ultimately improve the stability of the enslaved LO. We have validated these theoretical insights using numerical simulations of noisy local oscillators and calculations of relevant stability metrics.

The results we have presented have not by any means exhausted the space of modifications to clock protocols available using this framework. For instance we have numerically demonstrated improved correction accuracy using nonuniform-duration \( T_R \) over a cycle, as well as long-term stability improvement using only the simplest case of uniform \( T_R \). These approaches may be combined to produce LOs with improved accuracy at the time of correction and improved long-term stability. In cases where the penalty associated with increasing \( T_R \) is modest (lower high-frequency cutoff), such composite schemes can provide substantial benefits as well, improving both frequency standard accuracy and stability. Other expansions may leverage the basic analytic formalism we have introduced; we have introduced the transfer functions \( |G(\omega)|^2 \) and \( G_R^2(\omega) \), but have assumed only the simplest form for the time-domain sensitivity function and fixed overall gain. However, it is possible to craft a measurement protocol to yield \( |G(\omega)|^2 \) that suppresses the dominant spectral features of the LO noise. We have observed that through such an approach one may reduce the impact of aliasing on clock stabilization, providing a path towards reduction of the so-called Dick limit in precision frequency references.

In the parameter regimes we have studied the relative performance benefits of the hybrid feedback approach are of metrological significance - especially considering they may be gained using only “software” modification without the need for wholesale changes to the clock hardware. We believe the approach may find significant impact in tight-SWAP applications such as space-based clocks where improving the LO quality is generally impossible due to system-level limitations. Note: While preparing this manuscript we became aware of related work seeking to employ covariance techniques to improve measurements of quantum clocks [24].

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SUPPLEMENTARY MATERIAL

Frequency-domain variance expressions for general measurement windows

Point-like realisations of the stochastic process $y(t)$ cannot be obtained experimentally. Instead, the LO frequency error can be measured by a method that produces integrated samples, denoted $\bar{y}_k$ and indexed in time by $k$:

$$\bar{y}_k \equiv \frac{1}{T_k} \int_{t_k}^{t_{k+1}} y(t) dt$$

(5)

where $T_k \equiv t_{k+1} - t_k$. $[t_k, t_{k+1}]$ is the time interval over which the $k$th sample is taken, and $y(t)$ is a sensitivity function capturing the extent to which LO fluctuations at some instant $t$ contribute to the measured outcome for that sample. The range of $y(t)$ is $[0, 1]$ and its domain is $t \in [0, T_k]$. The ideal case is the rectangular window case, where

$$y(t) = \begin{cases} 1 & \text{for } t \in [0, T_k] \\ 0 & \text{otherwise} \end{cases}$$

(6)

in which case $\bar{y}_k$ reduces to the time-average of $y(t)$ over the interval $[t_k, t_{k+1}]$.

The variance of $\bar{y}_k$, denoted $\sigma^2(k)$ and often called true variance [19], is equal to the expected value of $\bar{y}_k^2$, since $y(t)$ is assumed to be a zero-mean process:

$$\sigma^2(k) = \mathbb{E}[\bar{y}_k^2]$$

(7)

$$= \mathbb{E}\left[\frac{1}{T_k} \int_{t_k}^{t_{k+1}} y(t) dt \right]^2$$

(8)

Defining a normalised, time-reversed sensitivity function $\bar{y}(t_m - t) = y(t - t_m)/T_m$, where $y(t)$ is assumed to be time-reversal symmetric about $t_m$, the midpoint of $[t_k, t_{k+1}]$, we can express the integral as a convolution:

$$\sigma^2(k) = \mathbb{E}\left[\left( \int_{-\infty}^{\infty} y(t) \bar{y}(t_m - t) dt \right)^2 \right]$$

(9)

Expanding this expression gives

$$\sigma^2(k) = \mathbb{E}\left[ \int_{-\infty}^{\infty} y(t) \bar{y}(t_m - t) dt \int_{-\infty}^{\infty} y(t') \bar{y}(t_m - t') dt' \right]$$

(10)

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathbb{E}[y(t)y(t')] \bar{y}(t_m - t) \bar{y}(t_m - t') dt dt'$$

(11)

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} R_{yy}(\Delta t) \bar{y}(k_m - t) \bar{y}(k_m - t') dt dt'$$

(12)

where $R_{yy}(\Delta t)$ is the two-sided autocorrelation function and $\Delta t \equiv t' - t$. Substituting the Wiener-Khinchin result

$$R_{yy}(\Delta t) = F^{-1}\{S_{yy}(\omega)\}$$

(13)

gives

$$\sigma^2(k) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left( \frac{1}{2\pi} \int_{-\infty}^{\infty} S_{yy}(\omega)e^{i\omega(t-t')} d\omega \right) \bar{y}(t_m - t) \bar{y}(t_m - t') dt dt'$$

(14)

Defining the Fourier transform of $\bar{y}(t_m - t)$:

$$G_k(\omega) \equiv \int_{-\infty}^{\infty} \bar{y}(t_m - t) e^{i\omega t} dt$$

(15)

and substituting it into the above expression for $\sigma^2(k)$ gives

$$\sigma^2(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} S_{yy}(\omega) G_k(\omega) G_k^*(\omega) d\omega$$

(16)

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} S_{yy}(\omega) |G_k(\omega)|^2 d\omega$$

(17)

$$= \frac{1}{2\pi} \int_{0}^{\infty} S_y(\omega) |G_k(\omega)|^2 d\omega$$

(18)

where $|G_k(\omega)|^2$ is called the transfer function for the $k$th sample. The substitution of the one-sided PSD $S_y(\omega)$ for the two-sided PSD $S_{yy}(\omega)$ is possible because $|G_k(\omega)|^2$ is even. This result is similar to the convolution theorem, which states that $F\{f \ast g\} = F\{f\} \cdot F\{g\}$, where $\ast$ denotes a convolution and $f$ and $g$ are Fourier-invertible functions.

The Allan variance, the conventional measure of frequency standard instability, can be expressed analogously

$$A^2_y(y) = \frac{1}{2\pi} \int_{0}^{\infty} S_y(\omega) |G(\omega)|^2 d\omega$$

(19)
where the transfer function, for ideal Ramsey interrogation, is

$$|A G(\omega)|^2 = \frac{2 \sin^4 \left(\frac{\omega T_R/2}{2}\right)}{\omega^2 T_R^2}$$

(20)

where \(T_R\) lacks an index because the definition of the Allan variance assumes equal-duration interrogation bins \([19]\). The Allan variance calculated via this frequency-domain approach can be compared to its value via the time-domain approach, which consists of finding the variance of the difference between consecutive pairs of measurement outcomes:

$$A^2 \sigma^2_{\bar{y}}(y) = \frac{1}{2} \langle (\bar{y}_{k+1} - \bar{y}_k)^2 \rangle$$

(21)

where \(\bar{y}_k\) is the \(k\)th measurement outcome and \(\langle \cdots \rangle\) may indicate a time average or an ensemble average, depending on whether \(y(t)\) is assumed to be ergodic.

Deriving the pair covariance transfer function

In order to calculate covariances involving multiple measurement outcomes and obtaining a useful feedforward predictor, we need a way of capturing the correlations between different measurements in the frequency domain. Using the identity \(\sigma^2(A + B) = \sigma^2(A) + \sigma^2(B) + 2\sigma(A, B)\), we define a sum and a difference sensitivity function: \(g^+_{k,l}(t)\) and \(g^-_{k,l}(t)\), with respect to two measurements indexed \(k\) and \(l\). \(g^+_{k,l}(t)\) and \(g^-_{k,l}(t)\) are general functions of time with two regions of high sensitivity.

$$g^\pm_{k,l}(t) = \begin{cases} g(t-t_k^\pm), & \text{for } t \in [t_k^\pm, t_k^\pm] \\ \pm g(t-t_l^\pm), & \text{for } t \in [t_l^\pm, t_l^\pm] \\ 0, & \text{otherwise} \end{cases}$$

(22)

These time-domain sum and difference sensitivity functions have their corresponding frequency-domain transfer functions, defined as their Fourier transforms normalised by \(T_R^{k,l}\):

$$G^\pm_{k,l}(\omega) = \int_{-\infty}^{\infty} \left(\frac{g(t_m^\pm - t)}{T_R^{k,l}} \pm \frac{g(t_m^\pm - t)}{T_R^{l,l}}\right) e^{i\omega t} dt$$

(23)

Substituting this and the form of the true variance (18) into the variance identity above and rearranging terms gives the covariance of the two measurement outcomes

$$\sigma(\bar{y}_k, \bar{y}_l) = \frac{1}{2\pi} \int_0^{\infty} S_y(\omega) \left( |G^+_{k,l}(\omega)|^2 - |G^-_{k,l}(\omega)|^2 \right) d\omega$$

(24)

$$= \frac{1}{2\pi} \int_0^{\infty} S_y(\omega) \left| G^2_{k,l}(\omega) \right| d\omega$$

(25)

whereby \(G^2_{k,l}(\omega)\) is defined to be the pair covariance transfer function. Using (23), it is possible to recover known expressions for the true, Allan and sample variances pertaining to the LO, in terms of \(S_y(\omega)\) and the appropriate transfer functions.

Calculating variances for locked local oscillators

The standard measures for oscillator performance consider either a free-running LO or provide a means only to statistically characterize measurement outcomes under black-box conditions. Here we present explicit analytic forms for different measurements of variance in the presence of feedback locking.

We initially make the link between LO and LLO variances via a time-domain treatment. Consider the trajectory of the same frequency noise realisation \(y(t)\) in the cases of no correction, \(y^{LO}(t)\) and correction, \(y^{LLO}(t)\). The relation between these two cases of \(y(t)\) is

$$y^{LLO}(t) = y^{LO}(t) + \sum_{k=1}^n C_k$$

(26)

where \(C_k\) refers to the value of the \(k\)th frequency correction applied to the LO, \(n\) of which have occurred before time \(t\).

Under traditional feedback, each correction is directly proportional to the immediately preceding measurement outcome: \(C_k = w_k y^{LLO}(t)\), where \(w_k\) is correction gain. Since \(y^{LLO}(t)\) is calculated by convolving \(y^{LLO}(t)\) with a sensitivity function pertaining to the measurement parameters, (26) is a recursive equation in general. It is possible to cancel all but one of the recursive terms by setting the correction gain equal to the inverse of the average sensitivity \(\bar{g}_k \equiv \int_0^{T_R} g(t)/T_R e^{i\omega t} dt\) of the preceding measurement, i.e. \(w_k = -\bar{g}_k^{-1}\), where the minus sign indicates negative feedback. With this constraint we can write

$$y^{LLO}(t) = y^{LO}(t) - \bar{g}_k^{-1} y^{LLO}(t)$$

(27)

and for a Ramsey interrogation and measurement with negligibly short pulses, \(\bar{g}_k = 1\).

The frequency variance of an LLO can be found straightforwardly, by substituting (26) into the definition of frequency variance, with the additional substitution of (27) for the particular case of traditional feedback:
\[ \text{Var}[\hat{y}_{LLO}(t)] = \langle \hat{y}_{LLO}(t)^2 \rangle - \langle \hat{y}_{LLO}(t) \rangle^2 \]  
(28)  
\[ = \left( \langle \hat{y}_{LO}(t) + \sum_{k=1}^{n} C_k \rangle \hat{y}_{LLO}(t) \right)^2 \]  
(29)  
\[ = \left( \langle \hat{y}_{LO}(t)^2 \rangle \hat{y}_{LLO}^2 \right) \]  
(30)  
\[ = \langle \hat{y}_{LO}(t)^2 \rangle + \frac{\sigma_{\hat{y}_{LO}}^2(n)}{\hat{y}_n} - \frac{2}{\hat{y}_n} \langle \hat{y}_{LO}(t) \hat{y}_{\hat{LLO}} \rangle \]  
(31)  
\[ = \langle \hat{y}_{LO}(t)^2 \rangle + \frac{\sigma_{\hat{y}_{LO}}^2(n)}{\hat{y}_n} - \frac{2}{\hat{y}_n} \sigma(\hat{y}_{LO}(t), \hat{y}_{\hat{LLO}}) \]  
(32)  

where the progression from (29) to (30) is valid for traditional feedback only, and \( \langle \hat{y}_{LLO}(t) \rangle = 0 \) by assumption and \( n \) indexes the last measurement before \( t \).

Although the LLO frequency variance under hybrid feedforward for more than a single cycle cannot be expressed in a closed non-recursive form, a consideration of a single cycle can provide a value for \( \langle \hat{y}_{LLO}(t)^2 \rangle \) in terms of covariance matrix elements, which in turn can be found by substituting (26) into the definition of the variance:

\[ \text{Var}[\hat{y}_{LLO}] = \frac{\langle \hat{y}_{LLO}(t)^2 \rangle}{\langle \hat{y}_{LLO}(t) \rangle^2} \]  
(33)  
\[ = \left( 1 + w_k^2 - w_k \frac{|F_k|^2}{F_k^T M_k F_k} \right)^{-1} \]  
(34)  

The true variance for an LLO can be found in a similar way by substituting (27) into the definition of true variance:

\[ \sigma_{\hat{y}_{LLO}}^2(k) = \text{Var}[\hat{y}_{LLO}^k] \]  
(35)  
\[ = \text{Var}[\hat{y}_{LLO}^k - \frac{\hat{y}_k}{\hat{y}_{k-1}} \hat{y}_{LLO}^{k-1}] \]  
(36)  
\[ = \sigma_{\hat{y}_{LLO}}^2(k) + \left( \frac{\hat{y}_k}{\hat{y}_{k-1}} \right)^2 \sigma_{\hat{y}_{LLO}}^2(k-1) \]  
(37)  
\[ - \frac{2\hat{y}_k}{\hat{y}_{k-1}} \sigma(\hat{y}_{LLO}^{k-1}, \hat{y}_{LLO}^k) \]  
(38)

where the appropriate forms of the measurement transfer function (18) and the pair covariance transfer function can be substituted in to express \( \sigma_{\hat{y}_{LLO}}^2(k) \) in terms of \( S_k(\omega) \).

The expected value of the LLO sample variance can be found by substituting (26) into the definition of the sample variance, producing a generic expression for traditional feedback (one measurement per cycle correction) and hybrid feedforward (multiple measurements per cycle):

\[ \text{E}[\sigma_{\hat{y}_{LLO}}^2[N]] = \frac{1}{N} \sum_{k=1}^{N} \left\{ \sigma_{\hat{y}_{LLO}}^2(k') + \frac{1}{N^2} \sum_{p'=1}^{N} \sum_{q'=1}^{N} \sigma(\hat{y}_{LLO}^{p'}, \hat{y}_{LLO}^{q'}) - \frac{2}{N} \sum_{l=1}^{N} \sigma(\hat{y}_{LLO}^{l'}, \hat{y}_{LLO}^l) \right\} \]  
(39)  
\[ = \frac{1}{N} \sum_{k=1}^{N} \left\{ \left( \sigma_{\hat{y}_{LLO}}^2(k') + \sum_{r=1}^{[k'/n]} \sum_{s=1}^{[k'/n]} \sigma(C_r, C_s) - 2\hat{y}_{k'} \sum_{u=1}^{[k'/n]} \sigma(\hat{y}_{LLO}^{u'}, C_u) \right) \right. \]  
\[ + \frac{1}{N^2} \sum_{p'=1}^{N} \sum_{q'=1}^{N} \sigma(\hat{y}_{LLO}^{p'}, \hat{y}_{LLO}^{q'}) + \sum_{p=1}^{[k'/n]} \sum_{q=1}^{[k'/n]} \sigma(\hat{y}_{LLO}^{k'}, C_r) \]  
\[ \left. - \frac{2}{N} \sum_{l=1}^{N} \sigma(\hat{y}_{LLO}^{l'}, \hat{y}_{LLO}^l) + \sum_{r=1}^{[k'/n]} \sum_{s=1}^{[k'/n]} \sigma(C_r, C_s) \right\} \]  
(40)  
\[ = \frac{1}{N} \sum_{k=1}^{N} \left\{ \left( \sigma_{\hat{y}_{LLO}}^2(k') + \sum_{r=1}^{[k'/n]} \sum_{s=1}^{[k'/n]} \sigma(C_r, C_s) - 2\hat{y}_{k'} \sum_{u=1}^{[k'/n]} \sigma(\hat{y}_{LLO}^{u'}, C_u) \right) \right. \]  
\[ + \frac{1}{N^2} \sum_{p'=1}^{N} \sum_{q'=1}^{N} \sigma(\hat{y}_{LLO}^{p'}, \hat{y}_{LLO}^{q'}) + \sum_{p=1}^{[k'/n]} \sum_{q=1}^{[k'/n]} \sigma(C_p, C_q) \]  
\[ \left. - \frac{2}{N} \sum_{l=1}^{N} \sigma(\hat{y}_{LLO}^{l'}, \hat{y}_{LLO}^l) + \sum_{r=1}^{[k'/n]} \sum_{s=1}^{[k'/n]} \sigma(C_r, C_s) \right\} \]  
(41)  

where in the case of hybrid feedback, \( N \) is defined to be total number of measurements and \( n \) is the number of measurements per cycle. The summation signs with unprimed indices are sums over whole cycles (of which there are
and the primed indices are sums over all \( N \) measurements. In general, \( E[\sigma_{y^{LLO}}^2[N]] \) contains recursive terms that cannot be concisely expressed in terms of the LO PSD \( S_y(\omega) \) and covariance transfer function \( G^2(\omega) \).

In the case of traditional feedback, the distinction between primed and unprimed indices disappears and the expression reduces to:

\[
E[\sigma_{y^{LLO}}^2[N]] = \frac{1}{N-1} \sum_{k=1}^{N} \left\{ \left( \sigma_y^{LLO}(k) + \bar{g}_k \sum_{i=1}^{k-1} \sum_{r=1}^{k-1} \sigma(C_r, C_s) - 2\bar{g}_k \sum_{u=1}^{k-1} \sigma(y_L^{LO}, C_u) \right) \\
+ \frac{1}{N^2} \sum_{p=1}^{N} \sum_{q=1}^{N} \left( \sigma(y_L^{LO}, y_L^{LO}) + \bar{g}_p \sum_{w=1}^{p-1} \sum_{x=1}^{q-1} \sigma(C_x, C_y) \right) \\
- \frac{2}{N} \sum_{l=1}^{N} \left( \sigma(y_L^{LO}, y_L^{LO}) + \bar{g}_k \sum_{y=1}^{k-1} \sum_{z=1}^{l-1} \sigma(C_y, C_z) \right) \right\} \tag{42}
\]

where each term can be expressed in terms of \( S_y(\omega) \) and \( G^2(\omega) \).

The LLO Allan variance can be found by substituting (27) into the definition of the Allan variance (21):

\[
A^2 \sigma_{y^{LLO}}^2(k) = \frac{1}{2} E[(\bar{y}_{k+1}^{LLO} - \bar{y}_k^{LLO})^2] \tag{43}
\]

\[
= \frac{1}{2} E \left[ \left( \frac{\bar{g}_k}{\bar{g}_{k-1}} - \frac{\bar{g}_{k+1}}{\bar{g}_k} \right)^2 \sigma_y^{LLO}(k) + \left( \frac{\bar{g}_k}{\bar{g}_{k-1}} \right)^2 \sigma_y^{LLO}(k-1) \right] \tag{44}
\]

\[
= \frac{1}{2 \bar{g}_k} \sigma(y_L^{LO}, y_L^{LO}) - 2 \left( 1 + \frac{\bar{g}_{k+1}}{\bar{g}_k} \right) \sigma(y_L^{LO}, y_L^{LO}) + \frac{2\bar{g}_k}{\bar{g}_{k-1}} \sigma(y_L^{LO}, y_L^{LO}) - 2 \left( 1 + \frac{\bar{g}_k}{\bar{g}_{k-1}} \right) \sigma(y_L^{LO}, y_L^{LO}) \tag{45}
\]
Appendix D

MATLAB code for Frequency Standard Simulation

This appendix includes the key scripts that constitute the numerical model for calculating, simulating and searching for feedforward protocols.

D.1 queue.m

```matlab
1 clear all
2 tstart=clock;
3 % ======== INITIAL VARIABLES ========
4 % the one that is stepped by q is replaced inside the loop
5 ensemble=100;
6 power=-1;  % dominant noise power law
7 b12=1e-3;  % low-frequency noise cutoff
8 b23=1e1;   % high-frequency noise cutoff
9 Tc=1;      % cycle time
10 Tr=0.1;   % interrogation (Ramsey) time
11 gran = 0.5e-1;  % time-domain granularity
12 duty=Tr/Tc;       % measurement duty cycle
13 gain=1;           % overall correction gain
14 measnum=10;       % number of simulated measurements
15 hff=0;            % hybrid feedforward toggle
16 overlap=1;        % overlapping hybrid feedforward toggle
17 averages=1;       % averaged measurements for integration time scan
18 fixed = 1;        % the scaling factor for the PSD
19 usecmat=1;        % FALSE to override the covariance matrix with own weightings
20 order='mdc';      % Defining cycle structure: mdc = ...
21    'measure-deadtime-correct', dmc = 'deadtime-measure-correct',dmdc ...
22    ='dead-measure-dead-correct'
23 bins=2;           % number of measurement bins in the protocol
24 seq_type='uniform';  % for FF: choices are 'uniform' or 'first'
25 scale=1;          % scale factor for the long first bin protocol
26
27 % ======== INITIALISE DATA VECTORS AND MATRICES ========
28 qstep=[0.1];     % specify the scan points
29 %qstep=[10/676.9];
30 qmax=numel(qstep);  % set the number of steps
```
%qmax=1;
qvec=[1:qmax]; % vector of steps
viewvec=[100]; % select the trace to see in figure 3

time=zeros(qmax,Tc*measnum/gran);
freqvarlo=zeros(qmax,Tc*measnum/gran);
freqvarfb=zeros(qmax,Tc*measnum/gran);
freqvarff=zeros(qmax,Tc*measnum/gran);
sampvarlo=zeros(qmax,measnum);
sampvarfb=zeros(qmax,measnum);
sampvarff=zeros(qmax,measnum);
allanvarlo=zeros(qmax,1);
allanvarfb=zeros(qmax,1);
allanvarff=zeros(qmax,1);
measvarlo=zeros(qmax,measnum);
measvarfb=zeros(qmax,measnum);
measvarff=zeros(qmax,measnum);
meanlo=zeros(qmax,1);
meanfb=zeros(qmax,1);
meanff=zeros(qmax,1);
meanlodev=zeros(qmax,1);
meanfbdev=zeros(qmax,1);
meanffdev=zeros(qmax,1);
measvarlo=zeros(qmax,measnum);
measvarfb=zeros(qmax,measnum);
measvarff=zeros(qmax,measnum);

for q=1:qmax
    duty=qstep(q); % allocate the stepped variable
    Tc=Tr/duty;
    Tr
    hff=0;
xcentrein=ones(100,1);

    str=['Starting FB scanpoint ',num2str(q),' of ',num2str(qmax)]
    [intime,infreqvarlo,infreqvarllo,insampvarlo,insampvarllo,inmeasvarlo,...
    inmeasvarllo,inallanvarlo,inallanvarllo,inmeanlo,inmeanllo,inylodev,...
    inylodev,xcentreout] = timedomain(fixed,power,b12,b23,Tc,gran,...
    ensemble,measnum,duty,gain,hff,overlap,averages,xcentrein,usecmat,...
    order,bins,scale,seq_type);

    time(q,:)=intime;

if size(insampvarlo,2)̸=size(sampvarlo,2)
    insampvarlo=[zeros(1,size(sampvarlo,2)-size(insampvarlo,2)) insampvarlo];
    insampvarlo=[zeros(1,size(sampvarlo,2)-size(insampvarlo,2)) insampvarlo];
    inallanvarlo=[zeros(1,size(allanvarlo,2)-size(inallanvarlo,2)) inallanvarlo];
    inallanvarlo=[zeros(1,size(allanvarlo,2)-size(inallanvarlo,2)) ...
    inallanvarlo];
inmeasvarlo=[zeros(1,size(measvarlo,2)-size(inmeasvarlo,2)) inmeasvarlo];
inmeasvarlo=[zeros(1,size(allanvarlo,2)-size(inmeasvarlo,2)) inmeasvarlo];
inmeasvarlo=[zeros(1,size(allanvarlo,2)-size(inmeasvarlo,2)) inmeasvarlo];
end

111
freqvarlo(q,:) = infreqvarlo;
freqvarfb(q,:) = infreqvarllo;
sampvarlo(q,:) = insampvarlo;
sampvarfb(q,:) = insampvarllo;
allanvarlo(q) = inallanvarlo;
allanvarfb(q) = inallanvarllo;
measvarlo(q,:) = inmeasvarlo;
measvarfb(q,:) = inmeasvarllo;
meanlo(q) = inmeanlo;
meanfb(q) = inmeanllo;
meaniodev(q) = inylodev;
meanfbdev(q) = inylldodev;

hff = 1;
xcentrein = xcentreout;
clear insampvarlo
clear insampvarllo
clear inallanvarlo
clear inallanvarllo
clear inmeasvarlo
clear inmeasvarllo
str = ['Starting HFF scanpoint ', num2str(q), ' of ', num2str(qmax)]
[intime, infreqvarlo, infreqvarllo, insampvarlo, insampvarllo, inmeasvarlo, ...
inmeasvarllo, inallanvarlo, inallanvarllo, inmeanlo, inmeanllo, inylodev, ...
inylldodev, xcentreout] = timedomain(fixed, power, b12, b23, Tc, gran, ...
ensemble, measnum, duty, gain, hff, overlap, averages, xcentrein, usecmat, ...
order, bins, scale, seq_type);

if size(insampvarlo,2) ≠ size(sampvarlo,2)
insampvarlo = [zeros(1, size(sampvarlo,2) - size(insampvarlo,2)) insampvarlo];
insampvarllo = [zeros(1, size(sampvarlo,2) - size(insampvarllo,2)) insampvarllo];
inallanvarlo = [zeros(1, size(allanvarlo,2) - size(inallanvarlo,2)) inallanvarlo];
inallanvarllo = [zeros(1, size(allanvarlo,2) - size(inallanvarllo,2)) ...
inallanvarllo];
inmeasvarlo = [zeros(1, size(measvarlo,2) - size(inmeasvarlo,2)) inmeasvarlo];
inmeasvarllo = [zeros(1, size(measvarlo,2) - size(inmeasvarllo,2)) inmeasvarllo];
end

freqvarlo(q,:) = (infreqvarlo + freqvarlo(q,:))./2;
freqvarff(q,:) = infreqvarllo;
sampvarlo(q,:) = (insampvarlo + sampvarlo(q,:))./2;
sampvarff(q,:) = insampvarllo;
allanvarlo(q) = (inallanvarlo + allanvarlo(q))./2;
allanvarff(q) = inallanvarllo;
measvarlo(q,:) = (inmeasvarlo + measvarlo(q,:))./2;
measvarff(q,:) = inmeasvarllo;

% meanlo(q) = (meanlo(q) + inmeanlo)./2;
meanff(q) = inmeanllo;
% meanlodev(q) = (meanlodev(q) + invlodev) / 2;
meanffdev(q) = invlodev;
end

% PLOT RESULTS %

figure(1) % Frequency variance vs time
hold on
plot(time', freqvarfb')
hold on
plot(time', freqvarff', 'r')
plot(time', freqvarlo', 'k')

xlabel('Time')
ylabel('Instantaneous variance')
title(['LLO Instantaneous variance vs. time. FF = ', num2str(hff), ', overlap = ', num2str(overlap)])

figure(2) % Sample variance vs measurement number

% plot(truevarlo', 'Color', [0 0.8 0], 'LineStyle', '- ', 'Marker', '*')
% hold on
% plot(truevarllo', 'Color', [0.5 0.8 0], 'LineStyle', '- ', 'Marker', '*')
plot(sampvarff(:, 2:end)', 'LineStyle', '-', 'Marker', '*')
hold on
plot(sampvarfb(:, 2:end)', 'LineStyle', '-', 'Marker', '+')
plot(sampvarlo(:, 2:end)', 'LineStyle', '-', 'Marker', 'o')
plot(measvarff(:, 2:end)', 'LineStyle', '-', 'Marker', '*', 'Color', 'r')
hold on
plot(measvarfb(:, 2:end)', 'LineStyle', '-', 'Marker', '+', 'Color', 'r')
plot(measvarlo(:, 2:end)', 'LineStyle', '-', 'Marker', 'o', 'Color', 'r')
% errorbar(sampvarllo(2:end)', devsigma(2:end)', 'Color', [0.5 0.8 0])
% errorbar(sampvarlo(2:end)', devsigmaLO(2:end)', 'Color', 'm')
xlabel('Number of measurements')
ylabel('Sample & measurement variance')
title(['LO and FF LLO sample & measure variances. FF = ', num2str(hff), ', overlap = ', num2str(overlap)])

figure(3) % Sample variance vs selected variable

% plot(truevarlo', 'Color', [0 0.8 0], 'LineStyle', '- ', 'Marker', '*')
% hold on
% plot(truevarllo', 'Color', [0.5 0.8 0], 'LineStyle', '- ', 'Marker', '*')
plot(qstep, sampvarff(:, viewvec)', 'LineStyle', '-', 'Marker', '*')
hold on
plot(qstep, sampvarfb(:, viewvec)', 'LineStyle', '-', 'Marker', '+')
plot(qstep, sampvarlo(:, viewvec)', 'LineStyle', '-', 'Marker', 'o')
% errorbar(sampvarllo(2:end), devsigma(2:end), 'Color', [0.5 0.8 0])
figure(4) % Normalised sample variance vs selected variable

plot(truevarlo,'Color',[0 0.8 0],'LineStyle','-','Marker','*')
hold on
plot(truevarllo,'Color',[0.5 0.8 0],'LineStyle','-','Marker','*')
plot(qstep,sampvarff(:,viewvec)./sampvarlo(:,viewvec),'LineStyle','-','Marker','*')
hold on
plot(qstep,sampvarfb(:,viewvec)./sampvarlo(:,viewvec),'LineStyle','-','Marker','+')
hold on
errorbar(sampvarllo(2:end),devsigma(2:end),'Color',[0.5 0.8 0])
errorbar(sampvarlo(2:end),devsigmaLO(2:end),'Color','m')
xlabel('Selected variable')
ylabel('Sample variance (normalised to LO)')
title(['LO and FF LLO sample variances. FF = ',num2str(hff),', overlap = ... ',' ,num2str(overlap)])

figure(5)
semilogx(qstep,abs(meanlo),'Marker','o')
hold on
errorbar(qstep,abs(meanlo),meanlodev)
semilogx(qstep,abs(meanfb),'Marker','+')
errorbar(qstep,abs(meanfb),meanfbdev)
semilogx(qstep,abs(meanff),'Marker','*')
errorbar(qstep,abs(meanff),meanffdev)

figure(6) % Allan variance vs selected variable

interrogationstep=qstep*duty*Tc
loglog(interrogationstep,allanvarff,'LineStyle','-','Marker','*')
hold on
loglog(interrogationstep,allanvarfb,'LineStyle','-','Marker','+')
loglog(interrogationstep,allanvarlo,'LineStyle','-','Marker','o')
xlabel('Selected variable')
ylabel('Allan variance')
title(['LO and FF LLO Allan variances. FF = ',num2str(hff),', overlap = ... ',' ,num2str(overlap)])

figure(7) % Normalised Allan variance vs selected variable

plot(qstep,allanvarff/allanvarlo,'LineStye','-','Marker','*')
hold on
plot(qstep,allanvarfb./allanvarlo,'LineStyle','-','Marker','+')
xlabel('Selected variable')
ylabel('Allan variance (normalised to LO)')
title(['LO and FF LLO Allan variances. FF = ',num2str(hff),', overlap = ... ',' ,num2str(overlap)])
D.2 timedomain.m

```matlab
function [time, instlo, instllo, meansigmaLO, meansigma, truevarlo, truevarllo, ... 
aveallanvarlo, aveallanvarllo, yloave, ylloave, ylodev, yllodev, xcentreout] =
timedomain(fixed, power, boundary12, boundary23, T, gran, rep, measnum, duty, gain, ...
 ff, overlap, averages, xcentrein, usecmat, order, bins, scale, seq_type)

%=============== Define the Power Spectral Density ===============
% Low cutoff below which PSD has power law 'lowfpower', high cutoff above
% which PSD has high-f roll-off function
locked=1; % apply correction or not, more efficient than just setting ...
gain = 0

timemax=T*measnum; % length of time series in time units
fine=timemax/gran; % Number of grains in the time vector
%boundary12=10^-5;
% boundary23=cutoff;
%boundary01=10^-5;
batch=10000; % putting the ensemble in batches to save RAM
maxmatsize=5e7;
if batch>rep
    batch=rep;
    str=['Batch size reduced to ',num2str(batch)]
end
if measnum*batch/gran>maxmatsize
    reduce=(measnum*batch/gran/maxmatsize);
    batch=batch/reduce;
    str=['Batch size reduced by a factor of ',num2str(reduce)]
end
%============ Choose traditional feedback or hybrid feedforward ===========
%ff=1; % choose hybrid feedforward (1) or traditional feedback (0)
if ~ff
    overlap=0; % traditional feedback does not need a moving average flag
    bins=1; % traditional feedback only uses one bin
    scale=1;
end
```
analytic=1; % if FB, whether or not to calculate analytic

if (ff==1&&bins==1)||(ff==0&&bins>1)
    error('Mismatch between number of bins and feedback/feedforward ... setting') % prevent inconsistent inputs
end

if (ff>1&&overlap==1)
    error('You are trying to do a moving predictor with traditional ... feedback') % prevent inconsistent inputs
end

%============== Define the vectors in frequency and time ===============

if (strcmp(seq_type,'uniform')&&scale>1)
    error('You are trying to apply a scale factor to a uniform bin ... protocol') % prevent inconsistent inputs
end

if (~strcmp(seq_type,'uniform')&&scale==1&&ff==1)
    error('You are trying to apply unity scale factor to a first bin ... protocol') % prevent inconsistent inputs
end

if (~ff&&scale>1)
    error('You are trying to apply a scale factor to traditional feedback') ...
        % prevent inconsistent inputs
end

%============== Define the sensitivity function ===============

if ff
    int_times=zeros(bins+1,2);
    cycle_int_times=zeros(bins+1,2,bins);
    for j=1:bins
        if strcmp(seq_type,'uniform')
            if strcmp(order,'dmc')
                int_times(j,:)=[T*(j-duty),T*j];  % dmc
            elseif strcmp(order,'mdc')
                int_times(j,:)=[T*(j-1),T*(j-1+duty)];  % mdc
            elseif strcmp(order,'dmdc')
                int_times(j,:)=[T*(j-(1+duty)/2),T*(j-(1-duty)/2)];  %dmdc
            else
                error('Not a valid order of measurement, deadtime and correction')
            end
            elseif strcmp(seq_type,'first')
                if scale>1
                    if overlap
                        loopend=(bins+scale-1);
                    end
                end
            else
                error('You are trying to apply a scale factor to a uniform bin ... protocol') % prevent inconsistent inputs
            end
        end
    end
end

%% %================================================================%
else
    loopend=1;
end
for w=1:loopend
    if w≤scale % calculating what the inversion should be
        v=1;
    else
        v=w-scale+1;
    end
    if j==v
        if strcmp(order, 'dmc')
            cycle_int_times(j,:,w)=[T*(j-duty),T*(scale+j-1)];
        elseif strcmp(order, 'mdc')
            cycle_int_times(j,:,w)=[T*(j-1),T*(scale+j-2+duty)];
        elseif strcmp(order, 'dmdc')
            cycle_int_times(j,:,w)=[T*(j-(1+duty)/2),T*(scale+j-1-(1-duty)/2)];
        else
            error('Not a valid order of measurement, deadtime and correction')
        end
    elseif j<v
        if strcmp(order, 'dmc')
            cycle_int_times(j,:,w)=[T*(j-duty),T*(j)];
        elseif strcmp(order, 'mdc')
            cycle_int_times(j,:,w)=[T*(j-1),T*(j-1+duty)];
        elseif strcmp(order, 'dmdc')
            cycle_int_times(j,:,w)=[T*(j-(1+duty)/2),T*(j-(1-duty)/2)];
        else
            error('Not a valid order of measurement, deadtime and correction')
        end
    elseif j>v
        if strcmp(order, 'dmc')
            cycle_int_times(j,:,w)=[T*(scale+j-1-duty),T*(scale+j-1)];
        elseif strcmp(order, 'mdc')
            cycle_int_times(j,:,w)=[T*(scale+j-2),T*(scale+j-2+duty)];
        elseif strcmp(order, 'dmdc')
            cycle_int_times(j,:,w)=[T*(scale+j-1-(1+duty)/2),T*(scale+j-1-(1-duty)/2)];
        else
            error('Not a valid order of measurement, deadtime and correction')
        end
    end
end
else
    if j==1
        if strcmp(order, 'dmc')
            int_times(j,:)=[T*(j-duty),T*(scale+j-1)];
        elseif strcmp(order, 'mdc')
            int_times(j,:)=[T*(j-1),T*(scale+j-2+duty)];
        elseif strcmp(order, 'dmdc')
            int_times(j,:)=[T*(j-(1+duty)/2),T*(scale+j-1-(1-duty)/2)];
        else
            error('Not a valid order of measurement, deadtime and correction')
        end
    end
else
    if j==1
        if strcmp(order, 'dmc')
            int_times(j,:)=[T*(j-duty),T*(scale+j-1)];
        elseif strcmp(order, 'mdc')
            int_times(j,:)=[T*(j-1),T*(scale+j-2+duty)];
        elseif strcmp(order, 'dmdc')
            int_times(j,:)=[T*(j-(1+duty)/2),T*(scale+j-1-(1-duty)/2)];
        else
            error('Not a valid order of measurement, deadtime and correction')
        end
    end
end
if strcmp(order, 'dmc')
    int_times(j,:) = [T*(scale+j-1-duty), T*(scale+j-1)];
elseif strcmp(order, 'mdc')
    int_times(j,:) = [T*(scale+j-2), T*(scale+j-2+duty)];
elseif strcmp(order, 'dmdc')
    int_times(j,:) = [T*(scale+j-1-(1+duty)/2), T*(scale+j-1-(1-duty)/2)];
else
    error('Not a valid order of measurement, deadtime and correction')
end
end
end
end

if scale > 1
    for w = 1:lopend
        if w <= scale % calculating what the test distance should be, long first bin ...
            only
            y(w) = w-1;
        else
            y(w) = 0;
        end
        cycle_int_times(bins+1,:,w) = [T*(bins+scale-1+y(w)), T*(bins+scale-1+y(w))+1e-12];
    end
end

if scale > 1
    for w = 1:lopend
        if w <= scale % calculating what the test distance should be, long first bin ...
            only
            y(w) = w-1;
        else
            y(w) = 0;
        end
        cycle_int_times(bins+1,:,w) = [T*(bins+scale-1+y(w)), T*(bins+scale-1+y(w))+1e-12];
    end
end

else
    if strcmp(order, 'dmc')
        int_times = [T*(1-duty), T; T, T+1e-12];
    elseif strcmp(order, 'mdc')
        int_times = [0, T*duty; T, T+1e-12];
    elseif strcmp(order, 'dmdc')
        int_times = [T*(1-duty)/2, T*(1+duty)/2; T, T+1e-12];
    else
        error('Not a valid order of measurement, deadtime and correction')
    end
    show_bins(int_times, 'feedback', 1);
    Tc = T;
else
    for b = 1:rep/batch
        end
% =========== SIMULATE NOISE, MEASUREMENT AND CONTROL ...

recmLLO=zeros(batch,floor(timemax/Tc*bins)); % matrix for recorded ...
measurement of LLO
recmLO=zeros(batch,floor(timemax/Tc*bins)); % matrix for recorded ...
measurement of LO
corrLLO=zeros(batch,floor(timemax/Tc*bins)); % matrix for corrections ...
applied to LLO
freq=logspace(-5,5,1000);

% find the index of freq corresponding to PSD roll-off boundary points
f12=1;
f23=numel(freq);
for f=1:numel(freq)
    if freq(f)<boundary12
        f12=f;
    elseif freq(f)≥boundary12&&freq(f)<boundary23
        f23=f;
    end
    if freq(f)*T<1e-3
        ft=f;
    else
        ft=1;
    end
end
f_low = freq(f12);
f_high=freq(f23);

str=['Starting batch ',num2str(b),' of ',num2str(rep/batch)]
[recylo,time,nf1,nf2,nf3,boundary3end,normtype,psdy,psdx]=...
colourednoise(fixed,batch,timemax,gran,power,boundary12,boundary23,T,duty,overlap);

% calculate the modified PSD for overlapping correction
figure(90)
loglog(freq,nf1(freq),'b')
hold on
loglog(freq,nf2(freq),'b')
loglog(freq,nf3(freq),'b')

if overlap
    nf1corr = @(x)(2*nf1(x).*{(sin(x.*pi*T*duty)./(x.*pi*T*duty)).^2 ...
                       -(2*cos(2*x.*pi*T) - cos(2.*x.*pi*T*(1-duty)) - cos(2.*x.*pi*T*(1+duty)) ...) ... ./((2*x.*pi.*T.*duty).^2));
    nf2corr = @(x)(2*nf2(x).*{(sin(x.*pi*T*duty)./(x.*pi*T*duty)).^2 ...
                       -(2*cos(2*x.*pi*T) - cos(2.*x.*pi*T*(1-duty)) - cos(2.*x.*pi*T*(1+duty)) ...) ... }
\[ \frac{1}{2} \pi T \text{duty} \right) \right)^2)); \\
\text{nf3corr} = @(x) \left( \frac{\sin(x \cdot \pi \cdot T \cdot \text{duty})}{x \cdot \pi \cdot T \cdot \text{duty}} \right)^2 - \left( \frac{2 \cdot \cos(2 \cdot x \cdot \pi \cdot T) - \cos(2 \cdot x \cdot \pi \cdot T \cdot (1 - \text{duty})) - \cos(2 \cdot x \cdot \pi \cdot T \cdot (1 + \text{duty}))}{(2 \cdot x \cdot \pi \cdot T \cdot \text{duty})^2} \right) \\
\right) \right)^2)); \\
\text{if } \text{strcmp}('\text{normtype}', '\text{area}') \\
\text{invalpha} = \text{integral}(\text{nf1corr}(x), 0, \text{boundary12}, '\text{ArrayValued}', true) + \text{integral}(\text{nf2corr}(x), \text{boundary12}, \text{boundary23}, '\text{ArrayValued}', true); \\
\text{elseif } \text{strcmp}('\text{normtype}', '\text{lowcutoff}') \\
\text{invalpha} = \text{nf1corr}(\text{f12}); \\
\text{elseif } \text{strcmp}('\text{normtype}', '\text{highcutoff}') \\
\text{invalpha} = \text{nf2corr}(\text{f23}); \\
\text{else} \\
\text{error('\text{Work out the noise type please.}')}) \\
\end{if} \\
\text{n1} = @(x) \text{nf1corr}(x) ./ \text{invalpha}; \\
\text{n2} = @(x) \text{nf2corr}(x) ./ \text{invalpha}; \\
\text{n3} = @(x) \text{nf3corr}(x) ./ \text{invalpha}; \\
\text{figure}(91) \\
\text{loglog}(\text{freq}, [\text{n1}(\text{freq}(1:12)) \text{n2}(\text{freq}(12:end))], 'm') \\
\text{recyllo} = \text{recylo}; \\
\text{corrylo} = \text{zeros}(\text{batch}, \text{size}(\text{recylo}, 2)); \\
\text{gee} = \text{zeros}(\text{T}/\text{gran}, 1); \\
\text{if } \text{strcmp('\text{order}', '\text{dmc}') \\
\text{gap} = 0; \\
\text{elseif } \text{strcmp('\text{order}', '\text{mdc}') \\
\text{gap} = \text{T} \cdot (1 - \text{duty}); \\
\text{elseif } \text{strcmp('\text{order}', '\text{dmdc}') \\
\text{gap} = \text{T} \cdot (1 - \text{duty}) / 2; \\
\end{if} \\
\text{freq} = \text{linspace}(1 / \text{timemax}, 1 / \text{gran}, \text{fine}); \\
\text{% ===== \text{CALCULATE HFF PREDICTOR COEFFICIENTS USING COVARIANCE MATRIX} ... \\
\text{if } \text{ff} \\
\text{if } \text{scale} > 1 \& \& \text{overlap} = 1
cyclelim=int_times(bins+1,1)/T; % as many corrections as T_seq/T

else
    cyclelim=1;
    cycle_int_times(:,:,1)=int_times(:,:,1);
    int_times
    if overlap==1
        y(1)=1; % what to do for uniform: 1=apply whitened PSD
    else
        y(1)=0;
    end
end

for w=1:cyclelim
    cycle_cmat(:,:,w)=intnoisecov(cycle_int_times(:,:,w),nf1,boundary12,nf2,...
        boundary23,nf3,psdy,psdx)

    for i=1:bins
        for j=1:bins
            V(i,j)=cycle_cmat(i,j,w);
            if abs(V(i,j))<1e-10 % getting rid of spurious small values
                V(i,j)=0;
            error('The correlations are too low to perform predictive feedforward')
            end
        end
        ET(i)=cycle_cmat(i,bins+1,w);
        if abs(ET(i))<1e-10 % getting rid of spurious small values
            ET(i)=0;
            error('The correlations are too low to perform predictive feedforward')
        end
    end
    F=cycle_cmat(bins+1,bins+1,w)

    if usecmat
        coeff(:,w)=ET.*sqrt(F./(ET*V*ET')).*gain; % use the ... covariance matrix to determine weightings
        % coeff(:,w)=coeff(:,w).*gain/(sum(coeff(:,w)));
        % further ... normalisation so the gain sum of coefficients is 1
    else
        coeff(:,w)=[-0.308;-0.3498;0.8601].*gain;% use ... predetermined fixed weightings
    end

    if ~(size(coeff,1)==bins)
        error('The number of weighting coefficients are not equal to the number ... of bins per cycle')
    end

    if overlap
        corrnum=bins; % as many corrections as measurements per cycle
    else
        corrnum=1; % one correction per cycle
end
else
correnum=1;
end
if ff
coeff
end
% ========= override coefficients to preset values ==========
% ============= EXTRACT MEASUREMENT OUTCOMES ===============
% Build the full time-domain sensitivity function
for t=1:T/gran
    for q=1:bins
        if t>=round(((int_times(q,1))/gran)&&t<(int_times(q,2))/gran)
            gee(t)=1;
        end
    end
end
sense=gee;
figure(76)
plot(gee,'+')
for m=2:measnum
    sense=vertcat(sense,gee);
end
prepmLO=reshape(recylo',T/gran,measnum,batch); % reshape the array ...
    for Ramsey averaging
% Match dimensions of traces and sensitivity function and multiply
if measnum>size(sense,2)
    sense=vertcat(sense,zerot(size(recylo,2)-size(sense,1),1));
elseif size(recylo,2)<size(sense,2)
    sense=sense(1:measnum);
end
sensemat=(sense*ones(size(sense,2),batch));
presense=reshape(sensemat,T/gran,measnum,batch);
measylo=prepmLO.*presense; % modulating the traces by the ...
    sensitivity function
recmLO=reshape(mean(measylo),measnum,batch)'./duty; % reshape and ...
recmLLO = recmLO; % initialise LLO measurement outcomes to LO outcomes

% =========== CALCULATE CORRECTIONS USING FB OR HFF ==============
if ff
    for m = 1:bins-1 % for k < n (first few measurements)
        recmLLO(:,m) = recmLLO(:,m) - sum(corrLLO,2);
        w = 1;
        recmLLO(:,1:m);
        coeff(bins-m+1:bins,1);
        corrLLO(:,m) = (recmLLO(:,1:m) * coeff(bins-m+1:bins,1));
    end
    for m = bins:measnum % for k ≥ n (rest of the measurements)
        recmLLO(:,m) = recmLLO(:,m) - sum(corrLLO,2);
        if size(coeff,2) > 1
            w = mod(m, bins) + 1;
        else
            w = 1;
        end
        recmLLO(:,1:m);
        coeff(1:bins,w);
        corrLLO(:,m) = (recmLLO(:,m-bins+1:m) * coeff(:,w));
    end
else
    for m = 1:measnum
        recmLLO(:,m) = recmLLO(:,m) - sum(corrLLO,2);
        corrLLO(:,m) = gain.* recmLLO(:,m);
    end
end

% apply the correction
for m = 1:measnum
    if m < measnum
        corrylo(:,numel(gee)*m+1:numel(gee)*(m+1)) = sum(corrLLO(:,1:m),2) * ones(1,numel(gee));
    end
    pastcorr(:,numel(gee)*(m-1)+1:numel(gee)*m) = corrLLO(:,m) * ones(1,numel(gee));
end
recyllo = recylo - corrylo; % apply corrections to the LLO
meanylo = mean(mean(recyllo)); % find the mean y_LLO value
meanylo = mean(mean(recylo)); % find the mean y_LO value

% apply averaging over contiguous measurements for variance calcs
if mod(measnum, averages) ≠ 0
    error('All values of the averaging set must be factors of the ...
          total number of measurements')
end
averecmLO=zeros(batch,measnum/averages);
averecmLLO=zeros(batch,measnum/averages);

for k=1:size(averecmLO,2)
    averecmLO(:,k)=mean(recmLO(:,(k-1)*averages+1:k*averages),2);
    averecmLLO(:,k)=mean(recmLLO(:,(k-1)*averages+1:k*averages),2);
end

% calculate sample variance per trace

for k=2:size(averecmLO,2)
clear meanelementLO
clear meanelementLLO
clear meanaveLO
clear meanaveLLO
for j=1:k
    meanelementLLO(:,j)=averecmLLO(:,j);
    meanelementLO(:,j)=averecmLO(:,j);
end
meanaveLLO=sum(meanelementLLO,2)./k;
meanaveLO=sum(meanelementLO,2)./k;
clear varelementLO
clear varelementLLO
for i=1:k
    varelementLLO(:,i)=(recmLLO(:,i)-meanaveLLO).^2;
    varelementLO(:,i)=(recmLO(:,i)).^2;
end
sampvarLLO(:,k)=sum(varelementLLO,2)/(k-1);
sampvarLO(:,k)=sum(varelementLO,2)/(k-1);
end

% calculate Allan variance per trace

if overlap||~ff
    for k=2:size(averecmLO,2)
        allanLLO(:,k-1)=(averecmLO(:,k)-averecmLO(:,k-1));
        allanLO(:,k-1)=(averecmLO(:,k)-averecmLO(:,k-1));
    end
elseif scale==1
    for k=1:floor(size(averecmLO,2)/bins)
        allanLLO(:,k)=averecmLO(:,1+k*bins)-averecmLO(:,1+(k-1)*bins);
        allanLO(:,k)=averecmLO(:,1+k*bins)-averecmLO(:,1+(k-1)*bins);
    end
    end
endif

% calculate average Allan variance over ensemble

if scale==1
    allanvarllo=sum((allanLLO.^2),2)/(2*size(allanLLO,2));
end
allanvarlo=sum((allanLO.^2),2)/(2*size(allanLO,2));
end

% ============= CALCULATE VARIANCE QUANTITIES =============

if batch==rep
    % yloave=mean(recylo); % time-average
    % ylloave=mean(recyllo); % average numerical instantaneous LLO ... variance

    % find numerical LO instantaneous var
    instlo=var(recylo);
    aveinstlo=mean(instlo);

    % find numerical LLO instantaneous var
    instllo=var(recyllo);
    aveinstllo=mean(instllo);

% find num LLO true var values
truevarllo=var(recmLLO);
truevarlo=var(recmLO);

% find num Allan var values
if scale==1
    allanvarllo=var(allanLLO)/2;
    allanvarlo=var(allanLO)/2;
end
% print the average Allan var values
% batchallanvarlo=mean(allanvarlo);
% devallanvarlo=sqrt(var(allanvarlo));
% batchallanvarllo=mean(allanvarllo);
% devallanvarllo=sqrt(var(allanvarllo));
else

    % yloave=zeros(size(recylo,2));
    % ylloave=zeros(size(recyllo,2));
    instlo=zeros(1,size(recylo,2));
    aveinstlo=0;
    instllo=zeros(1,size(recyllo,2));
    aveinstllo=0;
    truevarllo=zeros(1,size(recmLLO,2));
    truevarlo=zeros(1,size(recmLO,2));

    % find num Allan var values
    allanvarllo=var(allanLLO)/2;
    allanvarlo=var(allanLO)/2;

% % print the average Allan var values
aveallanvarlo=mean(allanvarlo);
devallanvarlo=sqrt(var(allanvarlo));
aveallanvarllo=mean(allanvarllo);
devallanvarllo=sqrt(var(allanvarllo));

end

% find numerical sample var LLO values
%batchvarsigma(b,:)=var(sampvarLLO);
batchmeansigma(b,:)=mean(sampvarLLO);
%batchdevsigma()=sqrt(varsigma);

% find numerical sample var LO values
%batchvarsigmaLO=var(sampvarLO);
batchmeansigmaLO(b,:)=mean(sampvarLO);
%batchdevsigmaLO=sqrt(varsigmaLO);

batchylo(b,:)=mean(recylo,2);
batchyllo(b,:)=mean(recyllo,2);

batchyloave(b)=mean(batchylo(b,:),2);
batchylloave(b)=mean(batchyllo(b,:),2);

if scale==1
batchallanvarlo(b)=mean(allanvarlo,2);
batchallanvarllo(b)=mean(allanvarllo,2);
end
end

% find numerical sample var LLO values
%varsigma=var(sampvarLLO);
meansigma=mean(batchmeansigma,1);
%devsigma=sqrt(varsigma);

% find numerical sample var LO values
%varsigmaLO=var(sampvarLO);
meansigmaLO=mean(batchmeansigmaLO,1);
%devsigmaLO=sqrt(varsigmaLO);

if scale==1
aveallanvarlo=mean(batchallanvarlo,2);
aveallanvarllo=mean(batchallanvarllo,2);
else
aveallanvarlo=zeros(size(batchmeansigma,1));
aveallanvarllo=mean(size(batchmeansigma,1));
end
yloave=mean(batchyloave);
ylloave=mean(batchylloave);

yloprepdev=reshape(batchylo,1,[]);
ylloprepdev=reshape(batchyllo,1,[]);
ylodev=sqrt(var(yloprepdev,0,2));
yllodev=sqrt(var(ylloprepdev,0,2));

figure(rep+1+ff)
hold off
hist(yloprepdev,ceil((rep-20)/100)+20)
ylonumel=hist(yloprepdev,ceil((rep-20)/100)+20);
hold on
scatter(mean(yloprepdev),[1],[],'r')
scatter(mean(yloprepdev)-ylodev,[1],[],'r','Marker','+')
scatter(mean(yloprepdev)+ylodev,[1],[],'r','Marker','+')
if ~ff
title(['Distribution of FB LLO trace means - mean ',num2str(yloave),' ...
' deviation ',num2str(ylodev),'. Total number of elements = ...','num2str(sum(ylonumel))])
else
title(['Distribution of Ismail-optimised LLO trace means - mean ...
' ',num2str(yloave),' deviation ',num2str(ylodev),'. Total number of ...
' elements = ',num2str(sum(ylonumel))])
end
figure(rep+3)
if ~ff
hist(yloprepdev,ceil((rep-20)/100)+20)
[xcentreout] = hist(yloprepdev,ceil((rep-20)/100)+20);
hold on
else
hist(yloprepdev,xcentrein,'Color','r')
xcentreout=xcentrein;
hold off
end
figure(rep)
hold off
hist(yloprepdev,ceil((rep-20)/100)+20)
ylonumel=hist(yloprepdev,ceil((rep-20)/100)+20);
hold on
scatter(mean(yloprepdev),[1],[],'r')
scatter(mean(yloprepdev)-ylodev,[1],[],'r','Marker','+')
scatter(mean(yloprepdev)+ylodev,[1],[],'r','Marker','+')
title(['Distribution of LO trace means - mean ',num2str(yloave),' ...
' deviation ',num2str(ylodev),'. Total number of elements = ...','num2str(sum(ylonumel))])

% ============= PLOT RESULTS =======================
%

figure(81)
plot(time,recylo(1,:), 'k')
hold on
plot(time,recylo(1,:), 'b')
plot(time,corrylo(1,:), 'r')

intimesize = size(time);
infreqvarlosize = size(instlo);
infreqvarllossiz e = size(instllo);
inmeansigmaLOsize = size(meansigmaLO);
inmeansigmaLLOsize = size(meansigma);
inmeasvarLOsize = size(truevarlo);
inmeasvarLLOsize = size(truevarllo);

% if size(recmLLO, 2)/bins>2
% figure(5)
% hold on
% if ff
% if overlap
% plot(allantime, allanvarllo, 'Color', [0 0.5 ... 0], 'LineStyle', '-', 'Marker', '*')
% else
% plot(allantime, allanvarllo, 'Color', [0 1 ... 0], 'LineStyle', '-', 'Marker', '*')
% end
% hold on
% plot(allantime, allanvarllo, 'Color', [0 0 1], 'LineStyle', '-', 'Marker', '*')
% xlabel('Number of measurements')
% ylabel('Allan variance')
% title('LO and FF LLO Allan variances')
% else
% plot(allantime, allanvarllo, 'Color', [0 0 ... 0], 'LineStyle', '-', 'Marker', '*')
% hold on
% plot(allantime, allanvarllo, 'Color', [0 0 1], 'LineStyle', '-', 'Marker', '*')
% xlabel('Number of measurements')
% ylabel('Allan variance')
% title('LO and FB LLO Allan variances')
% end
% end
%
% if ~locked
% figure(4)
% hold on
% plot(time, var(recylo), 'Color', [0 1 0])
D.3 intnoisevecov.m

function [ cov_matrix, allan_cov_matrix, f_ul] = intnoisevecov(int_times,...
   noise_function1,...
   boundary12,...
   noise_function2,...
   boundary23,...
   noise_function3,...
   psdy,psdx)

discrete=1;

freq1=logspace(-2,2,10000);

% intnoisevecov() returns a covariance matrix of random variables for noise
% integrated over the periods specified by [int_times], for a stationary,
% zero-mean gaussian noise process specified by noise functions and their
% boundaries.

% ** Note that frequency is always in units of 1/t. **

% [int_times]: (n x 2) matrix, where each row specifies the start and stop
% time of an interval over which noise is integrated. Note that this
% assumes noise g(t) sensitivity comes in rectangular pulses of unit
% height.

% [noise_function1]: the first noise function, extending from f = 0 to f =
% infinity if there are no further arguments, or f = boundary12.

% [boundary##]: frequency defining the transition between piecewise noise
% in segments # and #+1. Optional arguments which are only used if the next
% noise function is specified.

% [noise_function#]: noise function in segment #. Optional for # > 1.

% Example usage: c_mat = intnoisevecov([0,1;1,2], @(f)exp(-f.^2/(2*f_c^2)))
% Example usage: c_mat = intnoisecov([0,1;1,2], @(f)100, 1, @(f)100/f)
% if nargin > 6
%     error('intnoisecov:TooManyInputs', ...
%         'requires at most 6 optional inputs');
% end
if mod(nargin,2) ≠ 0
    error('intnoisecov:MissingInputs', ...
         'number of inputs should be even');
end

% Create flags for whether noise functions are used, whether a maximum
% frequency for integration is specified.
num_noise_segments = 1;
boundaries = [0;0];
% nf1 = @(f)(noise_function1(f));
% %nf1 = noise_function1;
%
% Several optional argument pairs
% switch nargin
%     case 4
%         num_noise_segments = 2;
%         if ~iscalar(boundary12)
%             error('intnoisecov:NonScalarInput', ...
%                 'input boundary12 must be scalar');
%             end
%         boundaries(1) = boundary12;
%         nf2 = fcnchk(noise_function2);
%         %nf2 = noise_function2;
%     case 6
%         num_noise_segments = 3;
%         if ~iscalar(boundary12)||~iscalar(boundary23)
%             error('intnoisecov:NonScalarInput', ...
%                 'inputs boundary12 and boundary23 must be scalar');
%             end
%         boundaries(1) = boundary12;
%         boundaries(2) = boundary23;
%         nf2 = @(f)(noise_function2(f));
%         nf3 = @(f)(noise_function3(f));
%     end
num_bins = size(int_times,1)-1;
% Build the covariance matrix element-by-element. Note that this is a
% symmetric matrix, so only need upper triangular elements
cov_matrix = zeros(num_bins+1);
allan_cov_matrix = zeros(num_bins+1);
granularity=1000;
fmin=-15;
fmax=log10(boundary23);
fplotting=logspace(fmin, fmax, granularity*(fmax-fmin));

figure(90)
loglog(freq1,nf1(freq1))
hold on
loglog(freq1,nf2(freq1))
loglog(freq1,nf3(freq1))

for i = 1:num_bins+1
  for j = 1:num_bins+1

    % Create shorthand variables for interval start/stop times
    t1 = int_times(i,1);
    t2 = int_times(i,2);
    t3 = int_times(j,1);
    t4 = int_times(j,2);

    % Define an ultra-low frequency boundary for numerical-integration
    % stability. Below this frequency, use Taylor approximation for
    % transfer function
    max_time_lag = max(abs(t4-t1), abs(t2-t3));
    % frequency always in units of 1/t
    % relative error in Taylor series should be < 1e-8.
    %
    min_time_lag = min(abs(t4-t2), abs(t3-t1));
    %
    if(min_time_lag == 0)
      min_time_lag = min(abs(t4-t3), abs(t2-t1));
      abs(t4-t3);
      abs(t2-t1);
    end

    if(min_time_lag == 0)
      Ti=abs(t2-t1)
      Tj=abs(t4-t3)
      error('intnoisecov: The minimum timescale is too small for ...
        MATLAB')
      min_time_lag = (1e-10)*max_time_lag;
    end

    %
    min_time_lag;

f_ul = 0.01/min_time_lag; % frequency always in units of 1/t

f_ultbigger=0;
bottom=0;
smaller=f_ul;

if f_ul > boundary23
    f_ultbigger=1;
    smaller=boundary23;
end

f_ultbigger=0;

% relative error in Taylor series should be < 1e-8.
f_ub = 10^(fmax-2); % integration upper bound

%f_min_time_lag;

if f_ul == 0
    error('intnoise: The minimum timescale is too small for ... MATLAB')
end

limh=floor(granularity*(log10(smaller)-fmin));
lims12=floor(granularity*(log10(boundary12)-fmin)); % change this ...
    for three-part noise
lims23=floor(granularity*(log10(boundary23)-fmin));

Htaylor_cutoff=fplotting(limh);
S_boundary12=fplotting(lims12);
S_boundary23=fplotting(lims23);

% Testing for the FID case

% Three cases: f_ul is below the first boundary (infinity if only
% one segment; f_ul is below the second boundary; f_ul is above the
% second boundary.

% Taylor coefficients
C1 = -0.5*((t4-t2)^2+(t3-t1)^2-(t4-t1)^2-(t3-t2)^2);
C2 = (1/24)*((2*pi)^2*(t4-t2)^4+(t3-t1)^4-(t4-t1)^4-(t3-t2)^4);
H_Taylor = @(f)(((C1 + C2*f.^2))/(t4-t3)/(t2-t1));

%./(pi*(t4-t3+t2-t1))

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\[ H_{\text{exact}} = \frac{1}{2\pi f^2} \left( \frac{1}{t_4-t_3} \frac{1}{t_2-t_1} \right) \left( \cos(2\pi f(t_4-t_2)) + \cos(2\pi f(t_3-t_1)) - \cos(2\pi f(t_4-t_1)) - \cos(2\pi f(t_3-t_2)) \right) \]

\[ H_f = \frac{1}{2\pi f} \left( \sin(2\pi f(t_3-t_1)) - \sin(2\pi f(t_3-t_2)) \right) \]

\[ H_{\text{Allan}} = \frac{1}{2\pi f^2} \left( \frac{1}{t_4-t_3} \frac{1}{t_2-t_1} \right) \left( \cos(2\pi f(t_4-t_2)) + \cos(2\pi f(t_3-t_1)) + \cos(2\pi f(t_4-t_1)) + \cos(2\pi f(t_3-t_2)) - 2\cos(2\pi f(t_4-t_1 - t_2)) - 2\cos(2\pi f(t_3-t_4/2 - t_2)) - 2\cos(2\pi f((t_1+t_2)/2 - t_3)) - 2\cos(2\pi f((t_1+t_2)/2 - t_4)) + 4\cos(2\pi f((t_1+t_2)/2 - (t_3+t_4)/2)) \right) \]

\[ ca_1 = -0.5 \left( (t_4-t_2)^2 + (t_3-t_1)^2 + (t_4-t_1)^2 + (t_3-t_2)^2 - 2( (t_4+t_3)/2 - t_2)^2 - 2( (t_4+t_3)/2 - t_1)^2 - 2( (t_1+t_2)/2 - t_3)^2 - 2( (t_1+t_2)/2 - t_4)^2 + 4( (t_1+t_2)/2 - (t_3+t_4)/2)^2 \right) \]

\[ ca_2 = \frac{1}{24} (2\pi)^2 \left( (t_4-t_2)^4 + (t_3-t_1)^4 + (t_4-t_1)^4 + (t_3-t_2)^4 - 2( (t_4+t_3)/2 - t_2)^4 - 2( (t_4+t_3)/2 - t_1)^4 - 2( (t_1+t_2)/2 - t_3)^4 - 2( (t_1+t_2)/2 - t_4)^4 + 4( (t_1+t_2)/2 - (t_3+t_4)/2)^4 \right) \]

\[ H_{\text{Allan Taylor}} = \frac{1}{(t_4-t_3)/(t_2-t_1)} \left( ca_1 + ca_2 f^2 \right) \]

\[ \text{if discrete} \]

\[ \text{if } (i==\text{num_bins+1} \&\& j==\text{num_bins+1}) \]

\[ \text{cov_matrix}(i,j) = H_f(\text{psdx}) \times \text{psdy}' ; \]

\[ \text{else if } (i==1 \&\& j==2) \]

\[ \text{cov_matrix}(i,j) = H_{\text{exact}}(\text{psdx}) \times \text{psdy}' ; \]

\[ \text{figure(69)} \]

\[ \loglog(\text{psdx},H_{\text{exact}}(\text{psdx}) \times \text{psdy},'rco') \]

\[ \text{hold on} \]

\[ \loglog(\text{psdx},\text{psdy},'bo') \]

\[ \loglog(\text{psdx},H_{\text{exact}}(\text{psdx}),'go') \]

\[ \text{else} \]

\[ \text{cov_matrix}(i,j) = H_{\text{exact}}(\text{psdx}) \times \text{psdy}' ; \]

\[ \text{end} \]

\[ [i \ j]; \]

\[ \text{else} \]

\[ \text{if } \neg(i==\text{num_bins+1}) \&\& \neg(j==\text{num_bins+1}) \]

\[ \text{if } f_{\text{ulbigger}}=0 \]

\[ \text{cov_matrix}(i,j) = \ldots \]
integral(@(x)(H_Taylor(x).*nf1(x)),0,boundary12) ...
+...
integral(@(x)(H_Taylor(x).*nf2(x)),boundary12,f_ul)+...
integral(@(x)(H_exact(x).*nf2(x)),f_ul,boundary23);

line=216;

elseif f_ulbigger==1

cov_matrix(i,j)= ...
integral(@(x)(H_Taylor(x).*nf1(x)),0,boundary12) ...
+...
integral(@(x)(H_Taylor(x).*nf2(x)),boundary12,boundary23);

line=224;
end

allan_cov_matrix(i,j)=...
integral(@(x)(H_Allan_Taylor(x).*nf1(x)),0,boundary12) ...
+...
integral(@(x)(H_Allan_Taylor(x).*nf2(x)),boundary12,f_ul) ...
+...
integral(@(x)(H_Allan(x).*nf2(x)),f_ul,boundary23);

elseif (i==num_bins+1&&j==num_bins+1)

cov_matrix(i,j)= ...
integral(@(x)(nf1(x)),bottom,boundary12) +...
integral(@(x)(nf2(x)),boundary12,boundary23);

allan_cov_matrix(i,j)=...
integral(nf1,bottom,boundary12) +...
integral(nf2,boundary12,boundary23);

line=243;
else

if f_ulbigger==0

cov_matrix(i,j)= ...
integral(@(x)(nf1(x)),bottom,boundary12) +...
integral(@(x)(nf2(x)),boundary12,f_ul)+...
integral(@(x)(H_f(x).*nf2(x)),f_ul,boundary23);

line=253;
elseif f_ulbigger==1

cov_matrix(i,j)= ...
    integral( @(x)(nf1(x)),bottom,boundary12) + ...
    integral( @(x)(nf2(x)),boundary12,boundary23);

    line=261;
end

if num_bins==1
    [t1,t2,t3,t4];
end
    end
end

for i=1:num_bins+1
    for j=1:num_bins+1

        % Set other half of off-diagonal entries

        if j>i
            cov_matrix(j,i) = cov_matrix(i,j);
            %cov_error(j,i)=cov_error(i,j);
            %cov_rel_error(j,i)=cov_rel_error(i,j);
            allan_cov_matrix(j,i) = allan_cov_matrix(i,j);
            %cov_error(j,i)=cov_error(i,j);
            %cov_rel_error(j,i)=cov_rel_error(i,j);
        end
    end
end

D.4 colourednoise.m

function [trace,time,nf1,nf2,nf3,b3end,normtype,psdoverlap,psdx] = ...
    colourednoise(fixed,ensemble,maxtime,mintime,power2,b12,b23,T,duty,overlap)
% INTENDED POWER SPECTRAL DENSITY
% specifies the power laws and rolloffs for a 3-part PSD

b01=1e-1; % lowest point of part 1
b12=1e-1; % boundary between parts 1 & 2
b23=1e1; % boundary between parts 2 & 3
b3end=1e1; % highest point of part 3

power1=0; % power law slope of part 1
power2=-1; % power law slope of part 2
power3=0; % power law slope of part 3

nf1=@(f)((b12/b23).^(power2).*(f./b12).^(power1)); % Constant chosen to be continuous with 2nd part of PSD
nf2=@(f)(f./b23).^(power2); % 2nd part defined so that PSD = 1 at boundary, prior to normalisation
nf3=@(f)(0); % high-f roll-off = 0 corresponds to a hard cut-off

spurson=0 % toggles whether to insert spurs symmetrically around 1/T

% NORMALISE INTENDED PSD
normtype='area';
if ~strcmp(normtype,'area')||strcmp(normtype,'lowcutoff')||strcmp(normtype,'highcutoff')
    error('Error: The type of normalisation you chose has not been coded yet.')
end

if strcmp(normtype,'area')
    normalpha=integral(@(x)(nf1(x)),b01,b12)+... % area under the PSD
        integral(@(x)(nf2(x)),b12,b23)+... % area under the PSD
        integral(@(x)(nf3(x)),b23,b3end,'ArrayValued',true);
elseif strcmp(normtype,'lowcutoff')
    normalpha=nf1(b12); % PSD evaluated at b12
elseif strcmp(normtype,'highcutoff')
    normalpha=nf2(b23); % PSD evaluated at b23
end

nf1=@(f)(nf1(f)./normalpha.*fixed);
nf2=@(f)(nf2(f)./normalpha.*fixed);
nf3=@(f)(nf3(f)./normalpha.*fixed);

alpha=integral(@(x)(nf1(x)),b01,b12)+... % with area normalisation, this should be equal to fixed
    integral(@(x)(nf2(x)),b12,b23)+... % with area normalisation, this should be equal to fixed
    integral(@(x)(nf3(x)),b23,b3end,'ArrayValued',true); % with area normalisation, this should be equal to fixed
%======== TIME AND FREQUENCY UNITS ===========

% mintime=0.5e-2; % set the shortest realised time interval, the highest ...
PSD element realised will be 1/(2*mintime)

% maxtime=1e2; % set the total trace duration

nyquist=1/2/mintime; % find the Nyquist rate with given sampling interval

tracelength=2*round(maxtime/mintime/2);

time=linspace(0,maxtime-mintime,tracelength);

freq=logspace(log10(b01),log10(b3end),tracelength); % a frequency vector ...
to plot the intended PSD

% locating the boundary points in the freq vector

f01=1;

f12=1;

f23=numel(freq);

f3end=numel(freq);

for f=2:numel(freq)
    if freq(f)>=b01&&freq(f-1)<b01
        f01=f;
    elseif freq(f)>=b12&&freq(f-1)<b12
        f12=f;
    elseif freq(f)>=b23&&freq(f-1)<b23
        f23=f;
    elseif freq(f)>=b3end&&freq(f-1)<b3end
        f3end=f;
    end
end

% work out the amount of aliasing

if nyquist<b23
    alphanyquist=integral(@(x)(nf1(x)),b01,b12)+...
    integral(@(x)(nf2(x)),b12,nyquist);
    alias=1+integral(@(x)(nf2(x)),nyquist,b23)/alphanyquist;
else
    alias=1;
end

%======== PLOT INTENDED AND REALISED PSD ==========

psdint=[nf1(freq(f01:f12-1)) nf2(freq(f12:f23-1)) ...
nf3(freq(f23:f3end))]/maxtime;

if numel(psdint)<numel(freq)
    freq=freq(1:numel(psdint));
end

%======== ENSEMBLE OF TIME-DOMAIN REALISATIONS ==========

offset='initial'; % options: mean (all traces have mean zero) or initial ...
(all traces start at zero)

trace=zeros(ensemble,tracelength);

% low frequency cutoff

fb=2*round(b12*maxtime)-1;
if fb<1
    fb=1;
end

% high frequency cutoff
fc=2*round(b23*maxtime)-1;
if fc>tracelength
    fc=tracelength;
end

% middle of frequency range
fmid=2*round(maxtime)-1;

% Generate the coefficients.
hfa = zeros ( 2 * tracelength, 1 );
hfa(1) = 1.0;

for i = 2 : tracelength
    hfa(i) = hfa(i-1) * ( 0.5 * (-power2) + ( i - 2 ) ) / ( i - 1 );
end
hfa(tracelength+1:2*tracelength) = 0.0;

fh = fft ( hfa );  % FFT the coefficients
fh = vertcat(zeros(fb-1,1).*fh(fb),fh(fb:fc),zeros(tracelength-fc,1)...  
             .*fh(fc+1:tracelength)) ; % truncate appropriately

% add spurs around 1/T
spur=max(abs(fh));
spurnum=11;
spurgap=100;
if spurson
    fh(fmid-spurgap*(spurnum-1)/2:spurgap:fmid+spurgap*(spurnum-1)/2)=spur;
end
for r=1:ensemble

    % Sample the white noise.
    wfa = sqrt(alpha) * randn ( tracelength, 1 );

    % Pad the array with zeros in anticipation of the FFT process.
    z = zeros ( tracelength, 1 );
    wfa = [ wfa; z ];

    % Perform the discrete Fourier transforms.
    fw = fft ( wfa );
% Truncate the vectors appropriately
fw = vertcat(fw(1:fc),zeros(tracelength-fc,1));

if size(fw,1)>size(fh,1)
    fw=fw(1:size(fh,1));
else if size(fw,1)<size(fh,1)
    fw=vertcat(fw,zeros(size(fh,1)-size(fw,1),1));
end

size(fw,1);
size(fh,1);

% Multiply the two complex vectors.
fw = fh.*fw;

% Scale to match the conventions of the Numerical Recipes FFT code.
fw(1) = fw(1) / 2.0;
fw(end) = fw(end) / 2.0;

% Pad the array with zeros in anticipation of the FFT process.
z = zeros ( tracelength - 1, 1 );
fw = [ fw; z ];

% Take the inverse Fourier transform.
x = ifft ( fw );

% Only the first half of the inverse Fourier transform is useful.
trace(r,:) = 2.0 * real ( x(1:tracelength) );

if strcmp(offset,'initial')
    trace(r,:)=trace(r,:)-trace(r,1);
elseif strcmp(offset,'mean')
    trace(r,:)=trace(r,:)-ones(1,tracelength).*mean(trace(r,:));
end

end

% ================ CALCULATE REALISED PSD =============

psd=mean(abs(fft(trace')').^2);
psd=2*psd(2:numel(psd)/2);

% preparing an x-vector to plot the realised PSD
psdx=[1:numel(psd)]./maxtime;

% locating the boundary points in the psdx vector
p01=1;
p12=1;
p23=numel(psdx);
p3end=numel(psdx);
for p=2:numel(psdx)
    if psdx(p)≥b01&&psdx(p-1)<b01
        p01=p;
    elseif psdx(p)≥b12&&psdx(p-1)<b12
        p12=p;
    elseif psdx(p)≥b23&&psdx(p-1)<b23
        p23=p;
    elseif psdx(p)≥b3end&&psdx(p-1)<b3end
        p3end=p;
    end
end

% renormalise the trace amplitudes so the area under their realised PSD is
% what we want, i.e. the variable 'area'
if strcmp(normtype,'area')
    psdarea=sum(psd);
elseif strcmp(normtype,'lowcutoff')
    psdarea=psd(p12);
elseif strcmp(normtype,'highcutoff')
    psdarea=psd(p23);
end

%fudge=1/sqrt(2);
trace=trace./sqrt(psdarea).*sqrt(fixed);
psd=mean(abs(fft(trace')).^2);
psd=2*psd(2:numel(psd)/2);
psdAA = psd./alias;
psdoverlap=psd.*((sin(psdx.*pi*T*duty)./(psdx.*pi*T*duty)).^2 - ...
    (2*cos(2*psdx.*pi*T) - cos(2.*psdx.*pi*T*(1-duty)) - ...
    cos(2.*psdx.*pi*T*(1+duty)))/(2*psdx.*pi*T*duty).^2).^overlap;
if ensemble>10 % prevents small ensembles having noisy PSDs displayed
    figure(30)
    loglog(freq,psdint)
    hold on
    loglog(psdx,psd,'r*-')
    loglog(psdx,psdAA,'ro'
    % loglog(psdx,psdoverlap,'+')
    xlabel('Fourier Frequency')
    ylabel('Power Spectral Density')
    title('Intended (blue solid) and Realised PSD, aliasing-compensated ...')
    (red stars) and uncompensated (red circles')
end
% =========== EXPORT DETAILS OF THE PSD ============
% work out the number of teeth in the f12-f23 band
bandvec=psdx(p12:p23);
bandteeth=size(bandvec);

% =========== CALCULATE DICK LIMIT ===============
dead = 0.5;
Tc = 2;

for h=1:1000
dickvector(h) = ((h/Tc*0.1).^(-1)).*(sin(2*pi*h*dead)/(2*pi*h)).^2;
end

figure(20)
plot(dickvector)
dick=(2/dead^2)*sum(dickvector)

% ============== PLOT EXAMPLE TRACES ==============
%showtrace=[1,10]; % a vector containing the indices of the traces to be ...
display
%figure(2)
%plot(time,trace(showtrace,:))

D.5 showbins.m

function [bin_points,hugosity] = show_bins(int_times,generate_type,cmatnum)
fineness=1;
fineness2=1;
square_lim=ceil(sqrt(fineness2));
int_times;

for r=[1:fineness]
    for p=[1:fineness2]
        clear bin_points
        hugosity=size(int_times,1);

        for i=[1:hugosity]
            for j=[1:2]
                int_times_mat(fineness,fineness2,i,j)=int_times(i,j);
            end
        end
    end
end
int_times;
% make the vector for the bin-step function
width=4*hugosity-2;

for d=2:width % Four points for each bin
    if (mod(d,4)==2) || (mod(d,4)==3)
        bin_points(d,1)=int_times(ceil(d/4),1);
    elseif (mod(d,4)==0)
        bin_points(d,1)=int_times(ceil(d/4),2);
    elseif mod(d,4)==1
        bin_points(d,1)=int_times(ceil(d/4)-1,2);
    end
    if (mod(d,4)==3) || (mod(d,4)==0)
        bin_points(d,2)=1;
    elseif (mod(d,4)==1) || (mod(d,4)==2)
        bin_points(d,2)=0;
    end
end

bin_points(1,1)=0;
bin_points(1,2)=0;

if p==1
    fignum=40+cmatnum;
    figure(fignum)
    if strcmp(generate_type,'parameterspace')
        subplot(2,1,1)
        hold off
        plot(bin_points(:,1),bin_points(:,2),'LineWidth',2);
        last_bin=(int_times(hugosity,1)-int_times(hugosity-1,1));
        for k=1:ceil(int_times(hugosity,1)/last_bin)
            % line([k*last_bin k*last_bin],[0 ... 1], 'LineStyle','--', 'Color','r')
        end
        plot(bin_points(:,1),bin_points(:,2),'LineWidth',2,'Color','b')
        xlim([-0.1*last_bin int_times(hugosity,1)+0.1*last_bin])
        ylim([-0.2 1.2])
        ff_length=int_times(hugosity,1);
        %set(gca,'XTick',[])
set(gca,'YTick',[0 1])
ylabel('g(t)','FontSize',24)
set(gca,'FontSize',16)

%hold on
% ...
plot(int_times(hugosity,1),0,'mx','LineWidth',2,'MarkerSize',10)

elseif strcmp(generate_type,'feedback')

subplot(2,1,2)
ylabel('g(t)','FontSize',24)
hold off
last_bin=int_times(2,1);
bib_size=int_times(2,1)-int_times(1,1);

%plot(bin_points(:,1)-k*bin_size,bin_points(:,2),'LineWidth',2,'Color','r');
plot(bin_points(:,1),bin_points(:,2),'LineWidth',2,'Color','r')

xlim([-0.1*bin_size last_bin+0.1*bin_size])
ylim([-0.2 1.2])

%plot(bin_points(width,1),0,'go','MarkerSize',10,'LineWidth',2)
%plot(int_times(hugosity,1),0,'mx','MarkerSize',10,'LineWidth',2)

ylabel('g(t)','FontSize',24)
set(gca,'YTick',[0 1])
xlabel('t (1/f_c)','FontSize',24)
set(gca,'FontSize',16)
title(['last_bin=',num2str(last_bin),', ... ' bin_size='num2str(bin_size)])

end

end
end
References

[1] Interview with David Wineland, for Annenberg Learner Physics Course Online.


