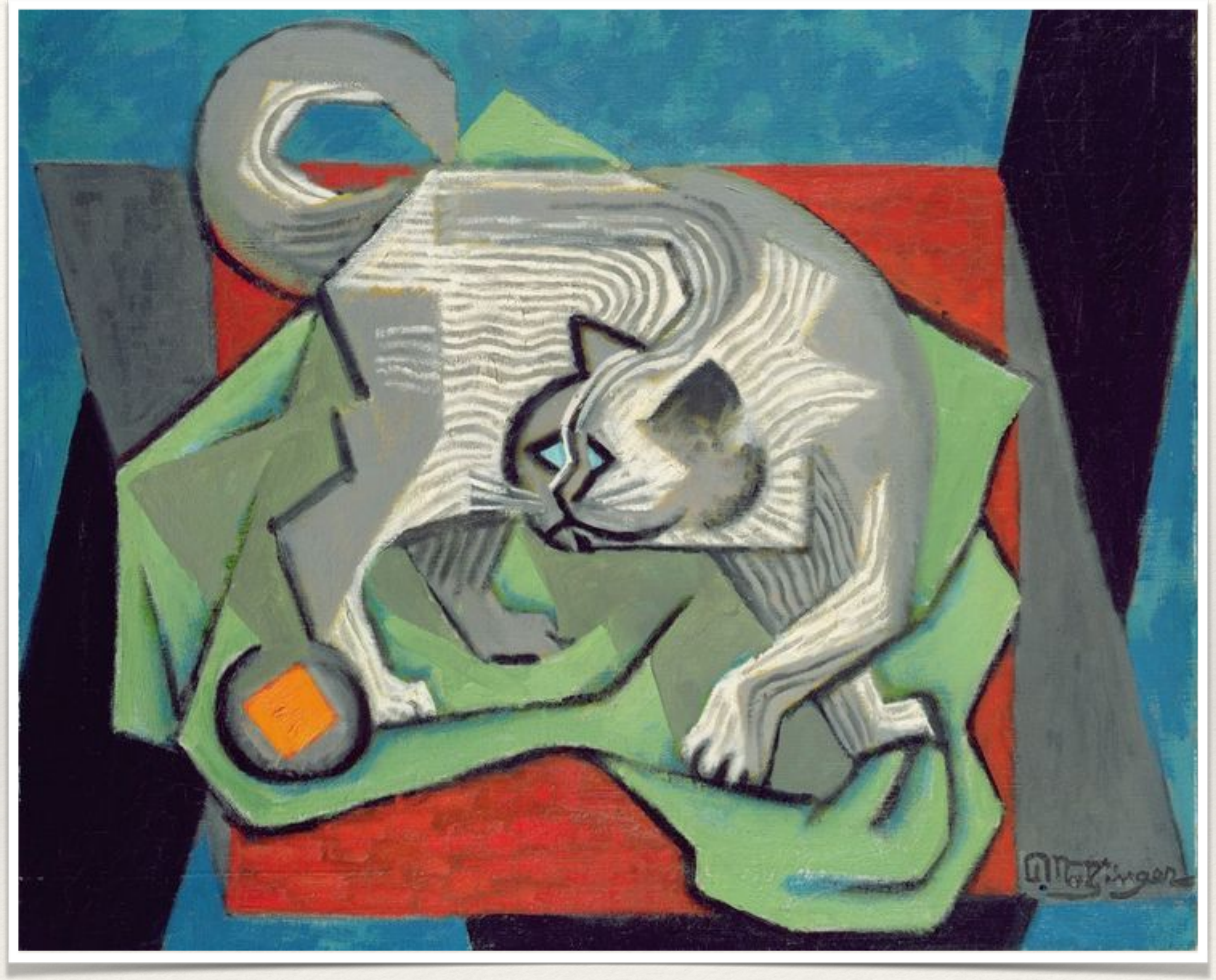
Prof. Steven Flammia

Quantum Mechanics

Lecture 15

Time-dependent perturbation theory;
The interaction picture.



A quick recap

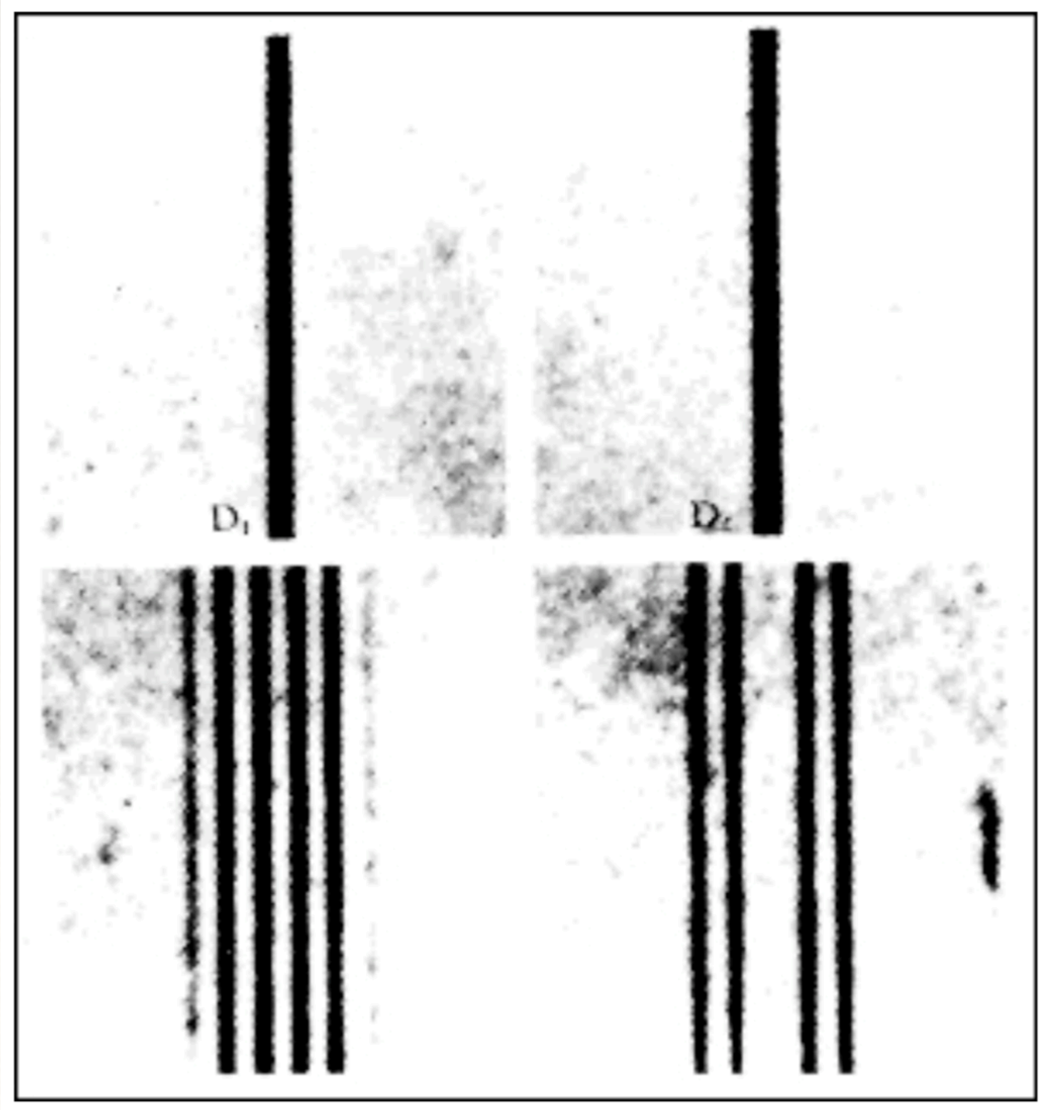
We derived the quantum Hamiltonian for a classical EM field: (Coulomb gauge)

$$H = \frac{-\hbar^2}{2m}\nabla^2 + \frac{i\hbar q}{mc}\mathbf{A}\cdot\nabla + \frac{q^2}{2mc^2}\mathbf{A}^2 + q\phi$$

$$A' = A + \nabla\Lambda$$
$$\phi' = \phi - \frac{1}{c}\frac{\partial\Lambda}{\partial t}$$

And, together with gauge invariance, we derived two phenomena:

Zeeman splitting



$$E_{n,l,m_l} = -\frac{me^4}{2\hbar^2 n^2} + \hbar\omega_L m_l$$

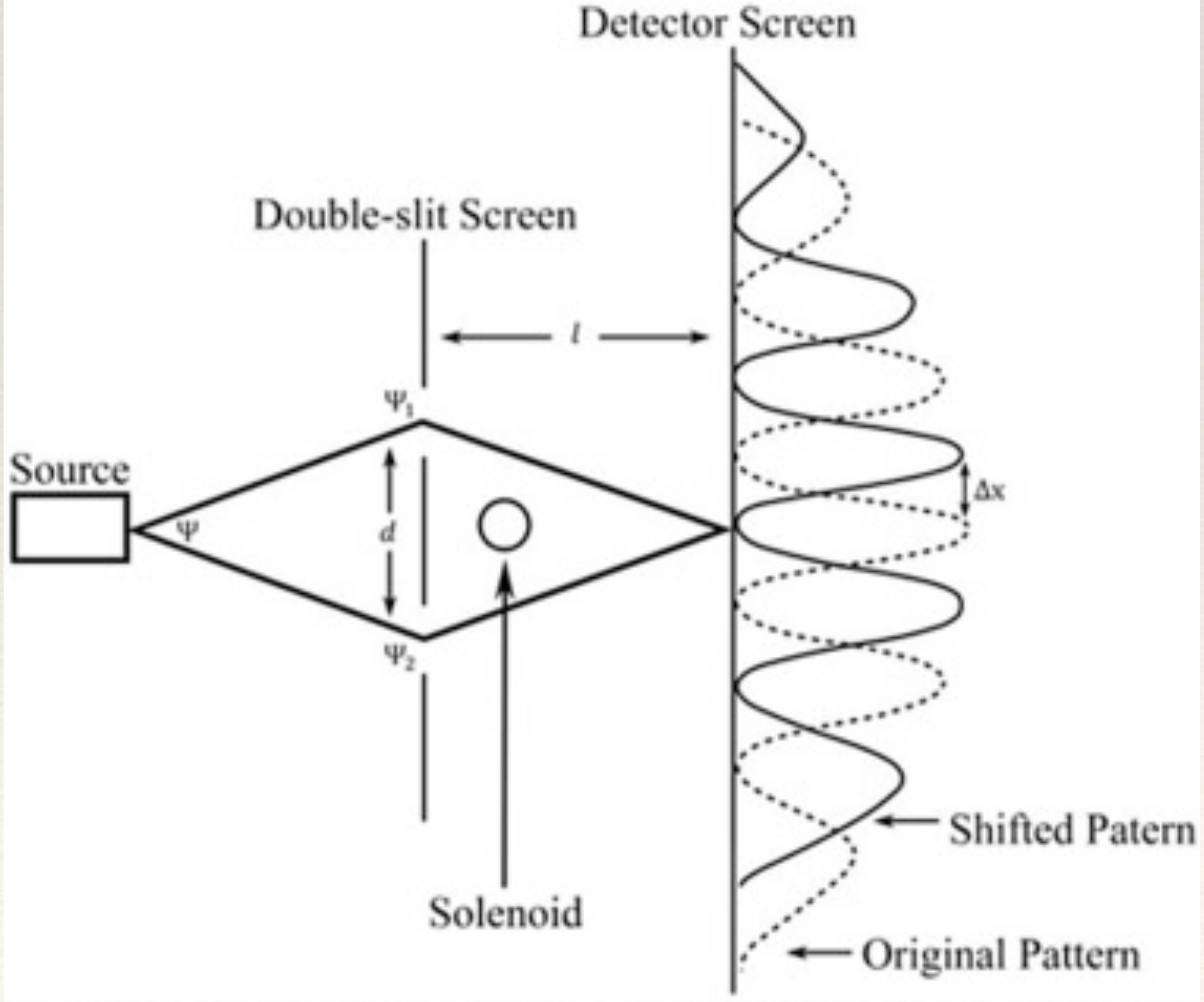
$$\omega_L = \frac{eB}{2mc}$$

Larmor frequency

Aharonov-Bohm effect

Phase shift based on flux through path

$$\Delta\gamma = \frac{e}{\hbar c}\Phi$$



Time-dependent perturbation theory

If we are interested in time dynamics of a system, we need more information from perturbation theory than what the time-independent case gives.

We allow our perturbing Hamiltonian to potentially depend explicitly on time and we make the following ansatz.

$$H(t) = H_0 + H_1(t)$$

total Hamiltonian

$$|\psi(0)\rangle = \sum_n |E_n^{(0)}\rangle\langle E_n^{(0)}|\psi(0)\rangle = \sum_n c_n(0)|E_n^{(0)}\rangle$$

initial state,
expanded in unperturbed eigenbasis

$$|\psi(t)\rangle = \sum_n c_n(t)\mathrm{e}^{-iE_n^{(0)}t/\hbar}|E_n^{(0)}\rangle$$

Time dynamics,
with c(t) containing the perturbing corrections to the bare evolution

$$|c_n(t)|^2$$

(c_n will be constant if $H = H_0$.)

The probability of being in the nth bare state at time t.

Using the Schrödinger equation

The Schrödinger equation tells us how the $c_n(t)$ evolve with time.

Schrödinger eq. $i\hbar\,|\dot{\psi}(t)\rangle = H\,|\psi(t)\rangle$

Ansatz state $|\psi(t)\rangle = \sum_n c_n(t) e^{-iE_n^{(0)}t/\hbar}\,|E_n^{(0)}\rangle$

Plug in H, use eigenvalue condition and chain rule:

$$i\hbar \sum_n \left(\dot{c}_n(t) e^{-iE_n^{(0)}t/\hbar} - \frac{iE_n^{(0)}}{\hbar} c_n(t) e^{-iE_n^{(0)}t/\hbar} \right) |E_n^{(0)}\rangle = \sum_n c_n(t) e^{-iE_n^{(0)}t/\hbar} (E_n^{(0)} + H_1)\,|E_n^{(0)}\rangle$$

Cancel 0th order energy term

$$i\hbar \sum_n \dot{c}_n(t) e^{-iE_n^{(0)}t/\hbar}\,|E_n^{(0)}\rangle = \sum_n c_n(t) e^{-iE_n^{(0)}t/\hbar} H_1\,|E_n^{(0)}\rangle$$

Isolate f component by inner product with $\langle E_f^{(0)}|$

$$i\hbar \sum_n \dot{c}_n(t) e^{-iE_n^{(0)}t/\hbar} \langle E_f^{(0)}\,|\,E_n^{(0)}\rangle = \sum_n c_n(t) e^{-iE_n^{(0)}t/\hbar} \langle E_f^{(0)}\,|\,H_1\,|\,E_n^{(0)}\rangle$$

Sum over δ function and simplify

$$i\hbar \dot{c}_f(t) = \sum_n c_n(t) e^{i\left(E_f^{(0)} - E_n^{(0)}\right)t/\hbar} \langle E_f^{(0)}\,|\,H_1\,|\,E_n^{(0)}\rangle$$

Perturbation series

We have derived a set of coupled differential equations for determining the evolution equations of the new amplitudes.

$$i\hbar\dot{c}_f(t) = \sum_n c_n(t)\mathrm{e}^{i\left(E_f^{(0)}-E_n^{(0)}\right)t/\hbar}\langle E_f^{(0)}\,|\,H_1\,|\,E_n^{(0)}\rangle$$

We now expand $c_n(t)$ as a perturbation series:

$$H_1 \to \lambda H_1 \qquad\qquad c_n(t) = c_n^{(0)} + \lambda c_n^{(1)} + \lambda^2 c_n^{(2)} + \ldots$$

$$i\hbar\left(\dot{c}_f^{(0)} + \lambda\dot{c}_f^{(1)} + \ldots\right) = \sum_n \left(c_n^{(0)} + \lambda c_n^{(1)} + \ldots\right)\mathrm{e}^{i\left(E_f^{(0)}-E_n^{(0)}\right)t/\hbar}\langle E_f^{(0)}\,|\,\lambda H_1\,|\,E_n^{(0)}\rangle$$

As with time-independent perturbation theory, we now equate terms at each order in λ to find self-consistent equations for the perturbative corrections.

0th order and initial conditions

Collecting terms at 0th order, we find

$$i\hbar\left(\dot{c}_f^{(0)} + \lambda \dot{c}_f^{(1)} + \ldots\right) = \sum_n \left(c_n^{(0)} + \lambda c_n^{(1)} + \ldots\right) \mathrm{e}^{i\left(E_f^{(0)} - E_n^{(0)}\right)t/\hbar} \langle E_f^{(0)} | \lambda H_1 | E_n^{(0)} \rangle$$

0th order equation: $\dot{c}_f^{(0)} = 0$

We need boundary conditions, so assume we initialize as follows.

Assume we start in an unperturbed eigenstate:

initial state: $|\psi(0)\rangle = |E_i^{(0)}\rangle \;\Leftrightarrow\; c_n(0) = \delta_{ni}$

This implies: $c_f(0) = c_f^{(0)}(0) + \lambda c_f^{(1)}(0) + \lambda^2 c_f^{(2)}(0)\ldots = \delta_{fi}$

$$\Leftrightarrow \quad c_f^{(0)} = \delta_{fi} \quad \text{and} \quad c_f^{(k)}(0) = 0 \text{ for } k \geq 1$$

1st order conditions

Collecting terms at 1st order, we find

$$i\hbar\left(\dot{c}_f^{(0)} + \lambda\dot{c}_f^{(1)} + \ldots\right) = \sum_n \left(c_n^{(0)} + \lambda c_n^{(1)} + \ldots\right)\mathrm{e}^{i\left(E_f^{(0)} - E_n^{(0)}\right)t/\hbar}\langle E_f^{(0)} | \lambda H_1 | E_n^{(0)}\rangle$$

1st order equation:

$$i\hbar\dot{c}_f^{(1)}(t) = \sum_n c_n^{(0)}\mathrm{e}^{i\left(E_f^{(0)} - E_n^{(0)}\right)t/\hbar}\langle E_f^{(0)} | H_1 | E_n^{(0)}\rangle$$

$$= \mathrm{e}^{i\left(E_f^{(0)} - E_i^{(0)}\right)t/\hbar}\langle E_f^{(0)} | H_1 | E_i^{(0)}\rangle$$

Use initial conditions to simplify

This can be integrated to obtain:

$$c_f^{(1)}(t) = \frac{-i}{\hbar}\int_0^t \mathrm{d}t'\,\mathrm{e}^{i\left(E_f^{(0)} - E_i^{(0)}\right)t'/\hbar}\langle E_f^{(0)} | H_1(t') | E_i^{(0)}\rangle$$

Schrödinger picture

We have been accustom to thinking of the state vector evolving in time:

$$|\psi_S(t)\rangle = U_S(t)\,|\psi_S(0)\rangle \qquad U_S(t) = \exp\left(-iHt/\hbar\right) \quad \text{(if H is time-independent.)}$$

We will call this the "Schrödinger picture" and label states and operators considered in this picture by a subscript S.

In the Schrödinger picture, time-evolution obeys:

$$i\hbar\dot{U}_S(t) = HU_S(t)$$

and expectation values (of time-independent operators) obey:

$$\frac{d}{dt}\langle\psi_S(t)\,|\,O_S\,|\,\psi_S(t)\rangle = \frac{i}{\hbar}\langle\psi_S(t)\,|\,[H, O_S]\,|\,\psi_S(t)\rangle$$

Heisenberg picture

In contrast to the Schrödinger picture, in the Heisenberg picture the operators evolve and the states remain fixed.

$$|\psi_H(t)\rangle = U_S(t)^\dagger|\psi_S(t)\rangle = |\psi_S(0)\rangle$$

$$\langle\psi_S(t)|O_S|\psi_S(t)\rangle = \langle\psi_S(0)|U_S(t)^\dagger O_S U_S(t)|\psi_S(0)\rangle = \langle\psi_H|U_S(t)^\dagger O_S U_S(t)|\psi_H\rangle = \langle\psi_H|O_H(t)|\psi_H\rangle$$

Here we have defined: $O_H(t) = U_S(t)^\dagger O_S U_S(t) = \mathrm{e}^{iHt/\hbar} O_S\, \mathrm{e}^{-iHt/\hbar}$

Heisenberg operator time evolution obeys:

$$\begin{aligned}\dot{O}_H &= \dot{U}_S(-t)O_S U_S(t) + U_S(-t)O_S\dot{U}_S(t)\\ &= \frac{i}{\hbar}\left(HU_S(-t)O_S U_S(t) - U_S(-t)O_S H U_S(t)\right)\\ &= \frac{i}{\hbar}[H, O_H]\end{aligned}$$

Interaction (Dirac) picture

The Schrödinger and Heisenberg pictures are "active" or respectively "passive" views of quantum evolution. The interaction picture combines features of both in a convenient way for time-dependent perturbation theory. Define:

$$|\psi_I(t)\rangle = \mathrm{e}^{iH_0 t/\hbar}|\psi_S(t)\rangle$$

Time evolution in the interaction picture proceeds as:

$$\begin{aligned} i\hbar|\dot{\psi}_I(t)\rangle &= -H_0\mathrm{e}^{iH_0 t/\hbar}|\psi_S(t)\rangle + \mathrm{e}^{iH_0 t/\hbar}i\hbar|\dot{\psi}_S(t)\rangle \\ &= -H_0\mathrm{e}^{iH_0 t/\hbar}|\psi_S(t)\rangle + \mathrm{e}^{iH_0 t/\hbar}(H_0 + H_1)|\psi_S(t)\rangle \\ &= \mathrm{e}^{iH_0 t/\hbar}H_1|\psi_S(t)\rangle \\ &= \mathrm{e}^{iH_0 t/\hbar}H_1\mathrm{e}^{-iH_0 t/\hbar}|\psi_I(t)\rangle \end{aligned}$$

Operator evolution in the interaction picture

We thus have:

$$|\psi_I(t)\rangle = \mathrm{e}^{iH_0t/\hbar}|\psi_S(t)\rangle \qquad i\hbar|\dot{\psi}_I(t)\rangle = \mathrm{e}^{iH_0t/\hbar}H_1\mathrm{e}^{-iH_0t/\hbar}|\psi_I(t)\rangle$$

Evolution of expected values of operators proceeds as:

$$\langle\psi_S(t)|O_S|\psi_S(t)\rangle = \langle\psi_I(t)|\mathrm{e}^{iH_0t/\hbar}\,O_S\,\mathrm{e}^{-iH_0t/\hbar}|\psi_I(t)\rangle = \langle\psi_I(t)|O_I|\psi_I(t)\rangle \qquad O_I := \mathrm{e}^{iH_0t/\hbar}\,O_S\,\mathrm{e}^{-iH_0t/\hbar}$$

Evolution of expected values of operators proceeds as:

$$\dot{O}_I = \frac{i}{\hbar}\left(\mathrm{e}^{iH_0t/\hbar}\,H_0O_S\mathrm{e}^{-iH_0t/\hbar} - \mathrm{e}^{iH_0t/\hbar}\,O_SH_0\mathrm{e}^{-iH_0t/\hbar}\right) = \frac{i}{\hbar}[H_0, O_I]$$

This suggests defining:

$$H_I = \mathrm{e}^{iH_0t/\hbar}H_1\mathrm{e}^{-iH_0t/\hbar} \qquad \Rightarrow \quad i\hbar|\dot{\psi}_I(t)\rangle = H_I|\psi_I(t)\rangle$$

Unitary evolution operator

In the interaction picture, H_I depends on time, complicating time evolution.

$$\dot{O}_I = \frac{i}{\hbar}[H_0, O_I] \qquad H_I = e^{iH_0 t/\hbar} H_1 e^{-iH_0 t/\hbar} \qquad i\hbar\,|\dot{\psi}_I(t)\rangle = H_I\,|\psi_I(t)\rangle$$

We can integrate the evolution equation as follows:

$$i\hbar \dot{U}_I(t) = H_I U_I(t) \;\Rightarrow\; U_I(t) = 1 - \frac{i}{\hbar}\int_0^t dt'\, H_I(t')U_I(t')\,, \quad U_I(0) = 1$$

To get a perturbative expression, we can iterate this:

$$U_I(t) = 1 - \frac{i}{\hbar}\int_0^t dt'\, H_I(t')\left(1 - \frac{i}{\hbar}\int_0^{t'} dt''\, H_I(t'')U_I(t'')\right) + \ldots$$

$$= 1 - \frac{i}{\hbar}\int_0^t dt'\, H_I(t') + \left(\frac{-i}{\hbar}\right)^2 \int_0^t dt'\, H_I(t') \int_0^{t'} dt''\, H_I(t'') + \ldots$$

Amplitude evolution

We can now derive the evolution equations for the $c_n(t)$ amplitudes.

$$|\psi_I(t)\rangle = \mathrm{e}^{iH_0 t/\hbar}|\psi_S(t)\rangle = \mathrm{e}^{iE_n^{(0)}t/\hbar}\sum_n c_n(t)\mathrm{e}^{-iE_n^{(0)}t/\hbar}|E_n^{(0)}\rangle = \sum_n c_n(t)|E_n^{(0)}\rangle \;\Rightarrow\; c_f(t) = \langle E_f^{(0)}|\psi_I(t)\rangle$$

Using the perturbative expansion for U_I(t), we find:

$$\begin{aligned}\langle E_f^{(0)}|U_I(t)|E_i^{(0)}\rangle &= \langle E_f^{(0)}|E_i^{(0)}\rangle - \frac{i}{\hbar}\int_0^t \mathrm{d}t'\,\langle E_f^{(0)}|H_I(t')|E_i^{(0)}\rangle + \ldots \\ &= \delta_{fi} - \frac{i}{\hbar}\int_0^t \mathrm{d}t'\,\mathrm{e}^{i(E_f^{(0)}-E_i^{(0)})t'/\hbar}\langle E_f^{(0)}|H_1(t')|E_i^{(0)}\rangle + \ldots\end{aligned}$$

This looks familiar! We can therefore see:

$$\left|c_f(t)\mathrm{e}^{-iE_f^{(0)}t/\hbar}\right|^2 = |c_f(t)|^2 = |\langle E_f^{(0)}|U_I(t)|E_i^{(0)}\rangle|^2$$