Macquarie University

Department of Physics

PHYS 304 Quantum Physics II

The content of this course, as outlined in the University Calendar, consists of more advanced aspects of quantum physics following on from the material presented in PHYS301.

CONTENT AND TEXTS

A. Das and A. C. Melissinos	*Quantum Mechanics, A Modern Introduction;*
J. J. Sakurai	*Modern Quantum Mechanics.*
R. L. Liboff	*Introductory Quantum Mechanics*

A copy of the first book is essential, the second and third are highly recommended reference texts.

STAFF

First half	6.5 weeks	Dr J Cresser (Office: E7A 318, Ext. 8951)
Second half	6.5 weeks	Dr. M Wheatland (Office: ??????)

ASSESSMENT

Assignment	30%
Final Take-home Exam	70%

The assignments will be approximately weekly. There is no minimum number of assignments required to be handed in, but of course, if you don't attempt the assignments, you will miss out on 30% of your final grade, and you will also miss out on valuable problem-solving experience. You will learn as much from the assignments as from lectures themselves.

COURSE CONTENT

The subject matter we will be aiming to cover will be drawn from the following list. Not every topic will necessarily be covered, and not all topics will be treated to the same depth.

First Half Semester (Dr J Cresser)

(1) **Introduction:** A brief introduction to the literature.
(2) **Mathematical formalism:** Hilbert space formulation, bra/ket vectors, operators, eigenvalues, eigenvectors and matrix representations, ensor products

of Hilbert space, continuous eigenvalue spectra and the Dirac delta function.

(3) **Basic postulates of quantum mechanics:** observables and operators, measurement in quantum mechanics, the state function and expectation values, quantum dynamics: time evolution and the Schrödinger equation, Heisenberg picture and Schrödinger picture, examples.

(4) **Symmetry in quantum mechanics:** operations on quantum system, symmetry operations and conservation laws in quantum mechanics.

(5) **Simple harmonic oscillator** as an important example.

(6) **Angular momentum in quantum mechanics:** angular momentum operators, orbital and spin angular momentum, spherical harmonics.

Second Half Semester (Dr M Wheatland)

(1) Particle spin, spin half particles and the Pauli spin matrices.

(2) Identical particles: symmetric and antisymmetric two-particle states, singlet and triplet states.

(3) Semiclassical treatment of electromagnetic field in quantum mechanics, the minimal coupling Hamiltonian, the Zeeman effect, dipole approximation, Rabi oscillations.

(4) Quantization of the electromagnetic field in a single mode cavity.

(5) Transition probabilities; time-dependent perturbation theory, stimulated emission and absorption.

(6) Time independent perturbation theory, the Stark effect, van der Waals forces.

* ORDER OF PRESENTATION

The co-ordinate representation

Wavefunctions, operators & their relationship to Dirac operators, the Schrodinger equation (SE)

Simple Harmonic oscillator (SHO)

Classical SHO & its probability distⁿ, importance of parabolic potential, time-dependent / time-independent SE

QUANTUM MECHANICS II

PHYS 304 2000
MACQUARIE UNIVERSITY

MIKE WHEATLAND

CONTENTS :

4. Identical particles

4.1 Exchange symmetry

4.2 Spin - statistics theorem

4.3 Elastic scattering of spinless Bosons

PHYS304 QUANTUM PHYSICS II 2000

I taught the second six weeks of this course: the first six weeks were taught by Jim Cresser. Jim covered the fundamentals of quantum mechanics, principally in the Dirac notation, and I taught four topics involving applications of the principles: the co-ordinate representation, the simple harmonic oscillator, angular momentum, and the treatment of identical particles. I would have liked to have covered more ground, but given the problems that I met (see below) I felt that it was wiser to restrict the course to a few topics.

The division of the course into two halves with separate lecturers was unsatisfactory, for both the students and myself. For the students, there was a lack of continuity in the style of presentation and in the material covered. From my own point of view (in the absence of printed lecture notes) I had no way of knowing exactly what was covered in the first six weeks. In the end I borrowed a set of hand-written lecture notes from one of the students, to determine what had been presented. Even then I found it difficult to get the students to acknowledge that something had been met before, or to accept as a starting point a result that Jim had arrived at. This situation would perhaps have been improved if there was a single textbook for the course, that covered most of the topics.

These are however structural problems. The fundamental problem with a course of this type is that the majority of the students do not have the requisite level of mathematical ability. I don't see any easy way around this problem. The use of the Dirac/Feynman approach is advantageous in that it reduces the mathematics to algebra, but it has the disadvantage that it is more abstract, and the students have difficulty with abstraction. I could complain a lot on this point, but I won't.

I took the approach of handing out weekly assignments, with just a few questions, with a view to monitoring the progress of the students. I felt that this approach was successful. I had regular visits from a number of the students seeking help with the assignments, and the marks on the assignments were reasonable. In lectures I asked a lot of questions of the students. The majority of them were answered by Martin Ams, who was on the right track about half of the time.

Regarding the exam, the marks were low. The students evidently found my part of the exam more difficult than Jim's, which is probably due to their having met the principles of quantum mechanics in this form before (in 301). Perhaps I made the exam too difficult, although I felt that since we had covered relatively few topics, it should be reasonably demanding. For the final lecture of the course (at the request of the students) I gave a summary lecture, which basically outlined what would be in the exam. I think most of the students must have ignored this.

I did not obtain a student assessment on this course, although I should have. The last weeks of the course were hectic for me and I simply forgot.

In summary I feel there were structural problems and a fundamental difficulty with the course. The structural problems could be solved, but the mathematical weakness of the students will always make a course at this level difficult to teach.

— Mike Wheatland

I. THE CO-ORDINATE REPRESENTATION :

We have learnt how to describe a QM system by a state vector in a Hilbert space, & have introduced the ideas of operators that act on these states.

A very useful method for studying many QM systems is to use the "co-ordinate representation", i.e. the representation in which the position eigenstates are the basis states.

Recall that an arbitrary state $|\Psi\rangle$ can be expanded in the basis vectors $|\mu\rangle$ of an operator $\hat{\Omega}$:

$$|\Psi\rangle = \sum_{\mu} a_\mu |\mu\rangle. \qquad (1)$$

The operator $\hat{\Omega}$ has eigenvalues ω_μ, i.e.

$$\hat{\Omega}|\mu\rangle = \omega_\mu |\mu\rangle.$$

The amplitudes a_μ appearing in (1) are obtained by taking inner products & using the orthonormality of the $|\mu\rangle$:

$$a_\mu = \langle \mu | \Psi \rangle$$

Physically the a_μ are probability amplitudes for observing a given eigenstate ω_μ :

$$P(\omega_\mu) = |a_\mu|^2 = |\langle \mu | \Psi \rangle|^2$$

If we are describing the state of a particle & $\hat{\underset{\sim}{x}}$ is the position operator $\hat{\underset{\sim}{x}}$, we have

$$P(\underset{\sim}{x}) = |\langle \underset{\sim}{x} | \Psi \rangle|^2 . \quad \circledast$$

the amplitudes $\langle \underset{\sim}{x} | \Psi \rangle$ may be considered to be a function of space & time,

Box important equ's.

$$\boxed{\Psi(\underset{\sim}{x}, t) = \langle \underset{\sim}{x} | \Psi \rangle ,}$$

which is the wavefunction for the particle. The physical interpretation of the wavefunction follows from $\circledast$: its squared modulus describes the probability of finding the particle at a certain position. More exactly $|\Psi|^2 d^3\underset{\sim}{x}$ ($= |\Psi|^2 dx dy dz$) is the probability of finding the particle in an infinitesimal volume ($dV = dx dy dz$) about $\underset{\sim}{x}$.

1.1 The Schrodinger equation

The co-ordinate representation is concerned with the determination of the wavefunction for the particle. How is this done?

If the time evolution of a system is assumed to be contained in the state vectors (i.e. the operators are assumed to be time-invariant, & the basis states are fixed), then (as Jim showed,) the QM equation of motion is

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \hat{H} |\Psi\rangle ,$$

where $\hat{H}$ is the Hamiltonian (energy) operator. (Jim called this the SE.) Taking the inner product with $\langle \underset{\sim}{x}|$ gives

$$i\hbar \frac{\partial}{\partial t}\langle \underset{\sim}{x}|\Psi\rangle = \langle \underset{\sim}{x}|\hat{H}|\Psi\rangle$$

$$= \int d^3\underset{\sim}{x}' \langle \underset{\sim}{x}|\hat{H}|\underset{\sim}{x}'\rangle\langle \underset{\sim}{x}'|\Psi\rangle,$$

where the RHS has been expanded in the basis states $|\underset{\sim}{x}'\rangle$. The quantity

$$H(\underset{\sim}{x},\underset{\sim}{x}') = \langle \underset{\sim}{x}|\hat{H}|\underset{\sim}{x}'\rangle$$

is chosen to have the form

$$H(\underset{\sim}{x},\underset{\sim}{x}') = \delta^3(\underset{\sim}{x}-\underset{\sim}{x}')\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]$$

where $\delta^3(\underset{\sim}{x}) = \delta(x)\delta(y)\delta(z)$ is the Dirac delta function, which Jim introduced, & $V = V(\underset{\sim}{x})$ is the potential energy of the particle, & ∇^2 is the laplacian. This choice cannot strictly be derived - although justifications can be given - & may be considered to be a law of nature. With this choice we have

$$i\hbar \frac{\partial}{\partial t}\langle \underset{\sim}{x}|\Psi\rangle = \tilde{H}\langle \underset{\sim}{x}|\Psi\rangle$$

i.e.

$$\boxed{i\hbar \frac{\partial \Psi}{\partial t} = \tilde{H}\Psi,}$$

where

$$\boxed{\tilde{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\underset{\sim}{x}),}$$

which is the "time dependent" Schrodinger equation, describing the evolution of the wavefunction of a particle.

In the co-ordinate representation $\tilde{H}$ plays the role of the Hamiltonian, or energy operator. In this representation operators are differential operators.

To understand the role of $\tilde{H}$ as an energy operator, we apply the standard technique of looking for separable solutions to the PDE at hand, i.e. we look for sol'ns of the form (lower case)

$$\Psi(\underset{\sim}{x}, t) = f(t)\,\psi(\underset{\sim}{x})$$

Substituting this into the time dependent SE gives

$$i\hbar \frac{\partial f}{\partial t} = \frac{1}{\psi}\tilde{H}\psi .$$

The RHS is a function of position only, & the LHS is a function of time only. Hence both must be constant, & we label the constant E:

$$i\hbar \frac{\partial f}{\partial t} = Ef \qquad (1)$$

$$\tilde{H}\psi = E\psi . \qquad (2)$$

Equ. (2) looks like an energy eigenfunction equation, & so we identify E as the energy eigenvalue for the eigenfunction ψ satisfying (2). This equation, which written out is

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\underset{\sim}{x})\right]\psi = E\psi$$

is called the time-independent Schrodinger equation, because time no longer appears explicitly. The solution to Eq. ① is $f = e^{-iEt/\hbar}$, & so we have constructed particular solutions

end of L11 → §110

$$\Psi_E(\underset{\sim}{x},t) = e^{-iEt/\hbar}\psi_E(\underset{\sim}{x})$$

Note $\hat{H}\Psi_E = E\Psi_E$

to the time-dependent S.E.. Note that $|\Psi_E|^2 = |\psi|^2$ which does not depend on time, & so these solutions are stationary.

These are the stationary states Tim introduced: $\langle \underset{\sim}{x}|E\rangle = \psi_E(\underset{\sim}{x},t)$

More general solutions (time-dependent solutions) to the SE, are obtained by summing the particular solutions:

$$\Psi(\underset{\sim}{x},t) = \sum_E c_E \Psi_E(\underset{\sim}{x},t)$$

$$= \sum_E c_E e^{-iEt/\hbar}\psi_E(\underset{\sim}{x}).$$

This expression is fully equivalent to an expansion of an arbitrary state of the particle in terms of its energy eigenstates:

$$|\Psi\rangle = \sum_E c_E |E\rangle$$

Taking the inner product of this equation with $|\underset{\sim}{x}\rangle$ yields the wavefunction version.

The procedure for solving the SE is first to look for stationary solutions, &

then to construct more general solns from the stationary ones. We will follow this procedure for an important example - the simple harmonic oscillator - shortly.

Before returning to the development of the co-ordinate representation, it is worthwhile to note how the SE differs when there are many particles. In that case the equation becomes

$$i\hbar \frac{\partial \Psi(\underset{\sim}{x}_1, \underset{\sim}{x}_2, \ldots, t)}{\partial t} = \sum_i -\frac{\hbar^2}{2m}\left\{\frac{\partial^2 \Psi}{\partial x_i^2} + \frac{\partial^2 \Psi}{\partial y_i^2} + \frac{\partial^2 \Psi}{\partial z_i^2}\right\}$$

$$+ V(\underset{\sim}{x}_1, \ldots)\Psi(\underset{\sim}{x}_1, \ldots, t)$$

where the $\underset{\sim}{x}_i$ describe the positions of the particles, & $V(\underset{\sim}{x}_1, \ldots)$ ~~is the total~~ describes the PE of the particles. The SE for a single particle is simple, & it is tempting to interpret it as describing a "wave in space" representing the particle. However, we see that when there are many particles the wavefunction depends on many variables, & cannot be interpreted as a wave with a certain amplitude in space.

$|\Psi|^2 d^3\underset{\sim}{x}_1 d^3\underset{\sim}{x}_2 \ldots d^3\underset{\sim}{x}_N$ is probability ...

1.2 Expectation values &. position, momentum operators

The expected value of the energy of the particle is

$$\langle E \rangle = \langle \Psi | \hat{H} | \Psi \rangle$$

$$= \iint \langle \Psi | \underset{\sim}{x} \rangle \langle \underset{\sim}{x} | \hat{H} | \underset{\sim}{x}' \rangle \langle \underset{\sim}{x}' | \Psi \rangle \, d^3\underset{\sim}{x} \, d^3\underset{\sim}{x}'$$

& using $H(\underset{\sim}{x}, \underset{\sim}{x}') = \langle \underset{\sim}{x} | \hat{H} | \underset{\sim}{x}' \rangle = \delta^3(\underset{\sim}{x} - \underset{\sim}{x}') \tilde{H}$

we have

$$\boxed{\langle E \rangle = \int \Psi^* \tilde{H} \Psi \, d^3\underset{\sim}{x}}$$

Note that if the system is in the stationary state $\Psi_E = e^{-iEt/\hbar} \psi_E$, then $\tilde{H} \Psi_E = E \Psi_E$ (since $\tilde{H} \psi_E = E \psi_E$), & hence

$$\langle E \rangle = E \int |\Psi|^2 d^3\underset{\sim}{x}$$

$$= E,$$

since $|\Psi|^2$ is a probability density.

What is the position operator $\hat{\underset{\sim}{x}}$ in the co-ordinate representation? Note that the "average" position of the particle must be

$$\langle \underset{\sim}{x} \rangle = \int \underset{\sim}{x} P(\underset{\sim}{x}) \, d^3\underset{\sim}{x},$$

but $P(\underset{\sim}{x}) = |\Psi|^2$, & so we have

$$\boxed{\langle \underset{\sim}{x} \rangle = \int \Psi^* \underset{\sim}{x} \Psi \, d^3\underset{\sim}{x}.}$$

By comparison with $\langle E \rangle$, this suggests that the position operator in this representation is just $\underset{\sim}{x}$, i.e. $\tilde{\underset{\sim}{x}} = \underset{\sim}{x}$, which means that the action of the operator is just multiplication by $\underset{\sim}{x}$. More formally it can be shown that

the correspondence with the operator $\hat{\underset{\sim}{x}}$ is

$$\langle \underset{\sim}{x} | \hat{\underset{\sim}{x}} | \underset{\sim}{x}' \rangle = \underset{\sim}{x}\, \delta^3(\underset{\sim}{x} - \underset{\sim}{x}')$$

(cf. the result for the Hamiltonian).

What is the momentum operator? This must be chosen so that the basic commutation relationships

$$[\hat{x}, \hat{p}_x] = [\hat{y}, \hat{p}_y] = [\hat{z}, \hat{p}_z] = i\hbar$$

hold. Let us choose $\tilde{p}_x = -i\hbar \frac{\partial}{\partial x}$ & consider the operation of the commutator on an arbitrary wavefunction in the co-ordinate representation:

$$[\tilde{x}, \tilde{p}_x]\, \Psi = (\tilde{x}\tilde{p}_x - \tilde{p}_x \tilde{x})\, \Psi$$

$$= -i\hbar x \frac{\partial \Psi}{\partial x} + i\hbar \frac{\partial}{\partial x}(x\Psi)$$

$$= i\hbar \Psi$$

& hence $[\tilde{x}, \tilde{p}_x] = i\hbar$ with this choice.

Also with this choice the Hamiltonian operator $\tilde{H}$ "looks like" the classical Hamiltonian for a particle:

$$\tilde{H} = \frac{-\hbar^2}{2m}\nabla^2 + V = \tilde{p}^2/2m + V.$$

Hence we conclude that

$$\boxed{\tilde{\underset{\sim}{p}} = -i\hbar\nabla}$$

is the momentum operator in the co-ordinate representation.

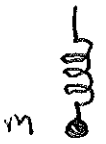
end of L2, 10/10

2. THE SIMPLE HARMONIC OSCILLATOR :

Before considering the QM simple harmonic oscillator we review the results for the classical system.

1.1 The classical SHO :

Consider a particle undergoing one-dimensional motion subject to a restoring force that is proportional to the displacement of the particle from its mean position. Then the equation of motion is



$$\frac{dp}{dt} = -kx,$$

where $p = mv = m\,dx/dt$ is the momentum & k is the "elastic constant" or "spring constant" (so called because this describes a mass oscillating on a spring). We have

$$\boxed{\frac{d^2x}{dt^2} = -\frac{k}{m}x = -\omega^2 x}$$

where $\omega^2 = k/m$, which has solution

$$x = A\sin(\omega t),$$

i.e. the mass undergoes oscillatory motion with angular frequency ω. The energy of the system is

$$E = \tfrac{1}{2}mv^2 + \tfrac{1}{2}kx^2 = \frac{p^2}{2m} + \tfrac{1}{2}m\omega^2x^2$$

(this is the "Hamiltonian" of the system). The term $V(x) = \tfrac{1}{2}m\omega^2x^2$ is the potential energy of the system.

We have seen that for each operator $\hat{\Omega}$ corresponding to an observable property of the particle there is a corresponding operator $\tilde{\Omega}$ in the co-ordinate representation. These operators are not equal: the formal correspondence is

$$\langle \underset{\sim}{x} | \hat{\Omega} | \underset{\sim}{x}' \rangle = \delta^3(\underset{\sim}{x} - \underset{\sim}{x}') \tilde{\Omega}$$

← (*) For every operator / state equation

$$|\Phi\rangle = \hat{A} |\Psi\rangle$$

there is a corresponding relationship for wavefunctions:

$$\Phi = \tilde{A} \Psi .$$

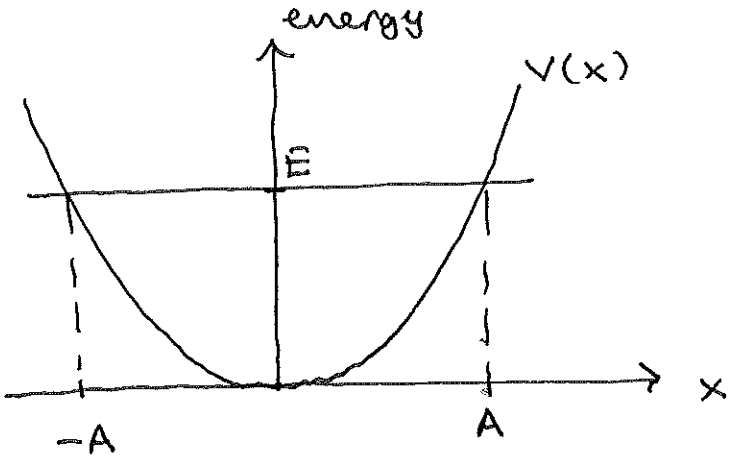
To see this, note that the operator/state equation implies

$$\begin{aligned} \langle \underset{\sim}{x} | \Phi \rangle &= \langle \underset{\sim}{x} | \hat{A} | \Psi \rangle \\ &= \int \langle \underset{\sim}{x} | \hat{A} | \underset{\sim}{x}' \rangle \langle \underset{\sim}{x}' | \Psi \rangle \, d^3\underset{\sim}{x}' \\ &= \tilde{A} \langle \underset{\sim}{x} | \Psi \rangle \end{aligned}$$

using the correspondence between operators. This, last relationship is $\Phi = \tilde{A} \Psi$, by the definition of the wavefunction.

As an example of the utility of the co-ordinate representation we next consider the solution of the SE for a parabolic potential (the simple harmonic oscillator, or SHO).

The energy diagram for the system is



For a given total energy E the particle oscillates between $\pm A$, where

$$\frac{1}{2}m\omega^2 A^2 = E \quad \Rightarrow \quad A = \left(\frac{2E}{m}\right)^{\frac{1}{2}}\frac{1}{\omega} = \left(\frac{2E}{k}\right)^{\frac{1}{2}}$$

Now consider the probability of finding the particle near a given point x. Clearly $P_{av}(x) = 0$ for $|x| > A$, because the particle is only permitted to be where $|x| \leq A$. For $|x| < A$ we have

$P_{av}(x)\,dx \propto$ fraction of time spent near x, averaged over many oscillations

& clearly $P_{av}(x) \propto \frac{1}{|v(x)|}$, because when the particle moves slowly it spends more time near a point.

We have $v = \frac{dx}{dt} = A\omega\cos(\omega t)$

so $|v| = \left|\frac{dx}{dt}\right| = A\omega\sqrt{1-\left(\frac{x}{A}\right)^2}$

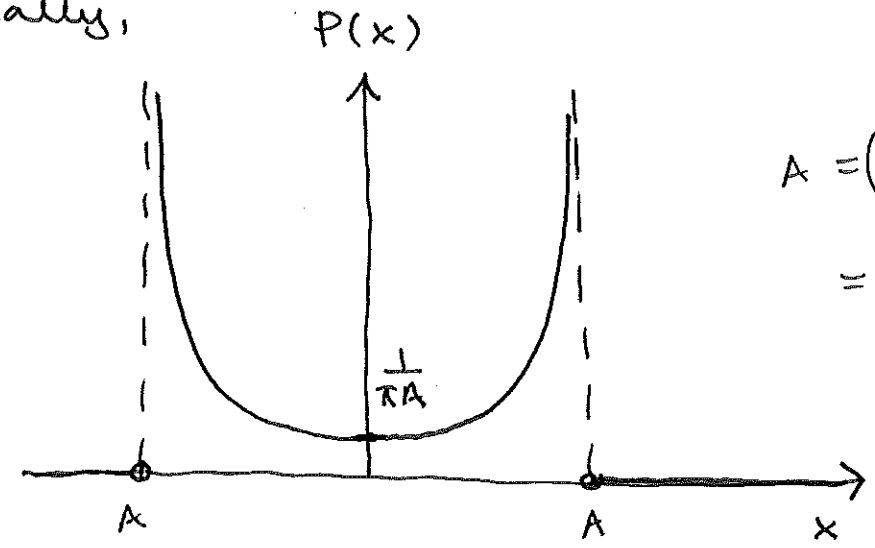
$$= \omega\sqrt{A^2 - x^2}$$

so $P_{av}(x) \propto \frac{1}{\omega\sqrt{A^2-x^2}}$

Normalising $\left(\int_{-A}^{+A} P(x)\,dx = 1 \right)$ leads to

$$P_{av}(x) = \frac{1}{\pi\sqrt{A^2 - x^2}} = \frac{1}{\pi\sqrt{\left(\frac{2E}{m\omega^2}\right) - x^2}} \quad \left(\frac{2E}{m\omega^2} = \frac{2E}{k}\right)$$

Graphically,



$$A = \left(\frac{2E}{m}\right)^{\frac{1}{2}} \frac{1}{\omega} = \left(\frac{2E}{k}\right)^{\frac{1}{2}}$$

The particle is more likely to be found near the turning points $x = \pm a$. The particle is never found where $|x| > \frac{2E}{m\omega^2}$. The energy of the particle is permitted to have any nonzero value.

Of course, it should be remembered that $P_{av}(x)$ is an average probability. The instantaneous probability of finding the classical system at x is given by

$$P(x,t) = \delta\left[x - A\sin(\omega t)\right]$$

where $\delta(x)$ is the Dirac delta function. In other words, the system is not probabilistic!

why? $\int_{-A}^{+A} P(x)\,dx = 1$

$P(x) = 0$ except where $x = A\sin(\omega t)$

end L3 11/10

1.2 THE QUANTUM-MECHANICAL SHO :

The time-dependent SE in 1-D is

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + V\Psi .$$

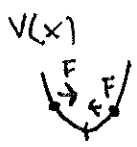
We wish to solve this equation for the choice of potential

$$\boxed{V = \tfrac{1}{2}m\omega^2 x^2 ,}$$

where ω is the "classical frequency". This choice of potential is of great practical significance, because it approximates an arbitrary potential in the neighbourhood of a stable equilibrium position. To see this, consider the expansion of an arbitrary potential about $x = x_0$:

$$V(x) = V(x_0) + (x-x_0)V'(x_0) + \tfrac{1}{2}(x-x_0)^2 V''(x_0) + \cdots$$

If $x = x_0$ is an equilibrium position then we require $F = -\left.\frac{dV}{dx}\right|_{x=x_0} = 0$. Also, if x_0 is a stable equilibrium, displacement of the particle a small distance from x_0 must lead to a force directed back towards x_0. In other words $V(x)$ must be concave up at x_0, i.e. $V''(x_0) > 0$. Hence our expansion becomes



$$V(x) = V(x_0) + \tfrac{1}{2}K(x-x_0)^2 + \cdots$$

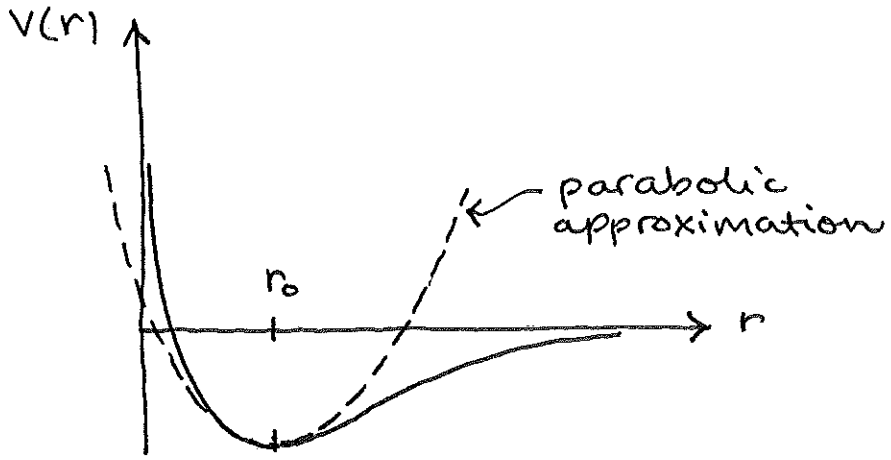
terms of order $(x-x_0)^3$

where $K > 0$.

If x_0 is chosen to be the origin & we take $V(x_0)=0$ (the zero-point for potential is arbitrary) then we have

$$V(x) = \tfrac{1}{2}Kx^2 + \cdots$$

& we see that the parabolic potential is the first approximation to any potential in the neighbourhood of a stable equilibrium. For example, the oscillations of atoms in a diatomic molecule are well described by the results for the SHO:



A second reason for the importance of the QM SHO is that the behaviour of most continuous physical systems, e.g. the oscillation of an EM field in a cavity, can be described as the superposition of infinitely many SHO's.

Returning to the problem at hand, we look first for stationary solutions (corresponding to energy eigenstates), i.e. we want to solve

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$

for $V = \frac{1}{2}m\omega^2x^2$. Some insight is gained by considering the behaviour of the solution for large $|x|$. First note that for a constant potential V_0 the solution for $V_0 > E$ is

$$\psi \sim e^{-\alpha x} \qquad (\text{for } x > 0)$$

where $\alpha = \frac{1}{\hbar}[2m(V_0 - E)]^{\frac{1}{2}}$. If we make the replacement $V_0 \to \frac{1}{2}m\omega^2x^2$ then for large x we expect $\alpha \sim \text{const.}\, x$ &

$$\psi \sim \exp(-\text{const.}\, x^2),$$

i.e. the wavefunction decays like a Gaussian. Adopting the usual form for a Gaussian,

$$\boxed{\psi = e^{-x^2/2a^2}}$$

For large $|x|$ the SE is

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} \simeq -\frac{1}{2}m\omega^2x^2 \qquad \circledast$$

We have

$$\frac{d\psi}{dx} = \frac{-x}{a^2}e^{-x^2/2a^2}$$

$$\frac{d^2\psi}{dx^2} = \frac{-1}{a^2}e^{-x^2/2a^2} + \frac{x^2}{a^4}e^{-x^2/2a^2}$$

$$\sim \frac{x^2}{a^4}e^{-x^2/2a^2}, \quad \text{for large } |x|$$

Substituting these expressions into $\circledast$ gives

$$\frac{-\hbar^2}{2m}\frac{x^2}{a^4}e^{-x^2/2a^2} \approx -\frac{1}{2}m\omega^2 x^2 e^{-x^2/2a^2}$$

$$\Rightarrow \boxed{a^2 = \frac{\hbar}{m\omega}}$$

We conclude that every wavefunction for the SHO is dominated by the same Gaussian decay for large distances from the centre of force. Close to the origin the solutions will differ.

end of L4

A general property of the solutions follows from the fact that $V(x)$ is symmetric $[V(-x) = V(x)]$. In a symmetric potential there is no reason for the particle to prefer one side of the potential to the other, & so

$$|\psi(-x)|^2 = |\psi(x)|^2.$$

The time-independent SE is a PDE with real coefficients, & so its solutions can be assumed to be real functions*. Hence

$$\psi(-x) = \pm\psi(x).$$

This tells us that the stationary states are either even or odd functions of x. With all of this knowledge, an obvious choice for a solution is

$$\psi(x) = f(x)\,e^{-x^2/2a^2},$$

where $f(x)$ is a polynomial that is odd or even. This form will ensure that the Gaussian behaviour dominates as $|x| \to \infty$.

* Not so for time-dependent SE

Now we solve the time-independent SE more rigorously. First, introduce a new co-ordinate:

$$\xi = \frac{x}{a} = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}} x,$$

scaling by our "decay length"

in which case the SE becomes (exercise)

$$\frac{d^2\psi}{d\xi^2} + \left(\frac{2E}{\hbar\omega} - \xi^2\right)\psi = 0 \qquad (*)$$

where $\psi = \psi[x(\xi)]$.

Exploiting our established knowledge of the solutions, we look for a solution of the form

$$\psi = e^{-\frac{1}{2}\xi^2} f(\xi),$$

where $f(\xi)$ is arbitrary. Substituting this into (*) leads to (exercise)

$$\frac{d^2f}{d\xi^2} - 2\xi\frac{df}{d\xi} + \left(\frac{2E}{\hbar\omega} - 1\right)f = 0. \qquad (**)$$

Consulting a book on orthogonal polynomials we see that the "Hermite" polynomials $H_n(\xi)$ satisfy

$$\frac{d^2H_n}{d\xi^2} - 2\xi\frac{dH_n}{d\xi} + 2nH_n = 0, \qquad (***)$$

with $n = 0, 1, \ldots$. These polynomials may be generated from

$$H_n = (-1)^n e^{\xi^2}\left(\frac{d}{d\xi}\right)^n e^{-\xi^2}$$

with $H_0 = 1$. The first few are:

$H_0 = 1$ $\qquad$ $H_3 = -12\xi + 8\xi^3$

$H_1 = 2\xi$ $\qquad$ $H_4 = 12 - 48\xi^2 + 16\xi^4$

$H_2 = -2 + 4\xi^2$ $\qquad$ $H_5 = 120\xi - 160\xi^3 + 32\xi^5$,

...

& notably they are alternately odd & even.

Comparing ⊛ & ⊛⊛ we see that the Hermite polynomials are candidate f's provided

$$\frac{2E}{\hbar\omega} - 1 = 2n$$

i.e. $\boxed{E = (n+\tfrac{1}{2})\hbar\omega}$ $\quad (n = 0, 1, \ldots)$

The corresponding wavefunctions are

$$\boxed{\upsilon_n = c_n e^{-\frac{1}{2}\xi^2} H_n(\xi) \qquad c_n = (\pi^{\frac{1}{2}} 2^n n!)^{-\frac{1}{2}}}$$

where

label them υ to distinguish from ψ

are normalisation constants. It turns out that these are the only normalisable solutions to the time-independent SE for the SHO potential. So we have solved the SE for the stationary states (energy eigenstates) of the system. We find that the allowed values of energy are quantized (cf. the classical SHO) with eigenvalues (eigenvalues)

$$\boxed{E_n = (n+\tfrac{1}{2})\hbar\omega, \quad n = 0, 1, \ldots}$$

Note that there is a lowest energy, $E_0 = \frac{1}{2}\hbar\omega$.

The energy eigenfunctions form an

orthonormal set, i.e.

$$\int_{-\infty}^{+\infty} d\xi\, v_m(\xi)\, v_n(\xi)\, d\xi = \delta_{m,n}$$

where

$$\delta_{m,n} = \begin{cases} 1 & \text{if } m=n \\ 0 & \text{if } m\neq n \end{cases}$$

is the Kronecker delta.

The wavefunctions in terms of our original variable x can be obtained from

$$|\psi_n(x)|^2 dx = |v_n(\xi)|^2 d\xi$$

(ensures normalisation is correct)

$$= |v_n[\xi(x)]|^2 \cdot \left|\frac{d\xi}{dx}\right| \cdot dx$$

& hence $$\psi_n(x) = v_n[\xi(x)] \cdot \left|\frac{d\xi}{dx}\right|^{\frac{1}{2}}$$

i.e. $$\psi_n(x) = (2^n n!)^{-\frac{1}{2}} \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2} H_n\left[\left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}} x\right],$$

which is formidable-looking. The orthonormality condition becomes

$$\int_{-\infty}^{+\infty} \psi_m(x)\, \psi_n(x)\, dx = \delta_{m,n} \,. \qquad (*)$$

Eq. (*) is a specific example of the general principle that eigenstates belonging to different eigenvalues of a particular operator are orthogonal. The connection with the Dirac formalism should be obvious by now: we begin with a set of orthonormal

energy eigenstates $|n\rangle$, i.e.

$$\langle m|n\rangle = \delta_{m,n}$$

i.e. $$\int d^3\underset{\sim}{x}\, \langle m|\underset{\sim}{x}\rangle\langle \underset{\sim}{x}|n\rangle = \delta_{m,n},$$

expanding in position states. Hence

$$\int d^3\underset{\sim}{x}\, \Psi_m^* \Psi_n = \delta_{m,n}$$

* then noting that the energy eigenstates have the form $\Psi_n = e^{-iE_nt/\hbar}\psi_n$, we recover ⊛.

end of L5 16/10

What do these solutions look like? The figure (from Bransden & Joachain) illustrates the first few eigenstates. A couple of points:

- The wavefunctions oscillate with approx. constant amplitude for $|\xi|$ less than some value, before decaying like Gaussians. The amplitude A of oscillation of the classical SHO provides an estimate for ξ_{max} (this is shown by the vertical lines in the RH panels). Specifically,

$$\tfrac{1}{2}m\omega^2A^2 = (n+\tfrac{1}{2})\hbar\omega$$

$$\Rightarrow A = (2n+1)^{\frac{1}{2}}\left(\frac{\hbar}{m\omega}\right)^{\frac{1}{2}}$$

$$\Rightarrow \xi_{max} = (2n+1)^{\frac{1}{2}}$$

However, there is a finite probability the particle will be found outside the

classically-permitted region.

- For large n we begin to see a correspondence between the QM probability & the classical average probability of finding the particle at a particular location (see RH panel figures, & the case $n=20$). For large n the fractional energy difference between states becomes small ($\frac{\hbar\omega}{E_n} \to 0$ as $n \to \infty$), so there is almost a continuum of energy levels, as in the classical case.

1.3 Recurrence relations:

The Hermite polynomials satisfy the "recurrence relations"

$$H_{n+1}(\xi) = 2\xi H_n(\xi) - 2n H_{n-1}(\xi)$$

$$\& \quad \frac{dH_n(\xi)}{d\xi} = 2n H_{n-1}(\xi)$$

Substituting $H_n(\xi) = c_n^{-1} e^{\frac{1}{2}\xi^2} v_n(\xi)$ leads to recurrence relations in the wavefunctions:

$$[2(n+1)]^{\frac{1}{2}} v_{n+1}(\xi) = 2\xi v_n(\xi) - (2n)^{\frac{1}{2}} v_{n-1}(\xi) \quad ①$$

$$\frac{dv_n(\xi)}{d\xi} = -\xi v_n(\xi) + (2n)^{\frac{1}{2}} v_{n-1}(\xi) \quad ②$$

Eq. ② can be rearranged to give

$$\left(\xi + \frac{d}{d\xi}\right) v_n(\xi) = (2n)^{\frac{1}{2}} v_{n-1}(\xi)$$

* using this formula to replace the last term on the RHS of ① gives

$$[2(n+1)]^{\frac{1}{2}} v_{n+1}(\xi) = 2\xi v_n(\xi) - \left(\xi + \frac{d}{d\xi}\right) v_n(\xi)$$

$$= \left(\xi - \frac{d}{d\xi}\right) v_n(\xi).$$

Hence we have established

$$\left(\xi + \frac{d}{d\xi}\right) v_n(\xi) = (2n)^{\frac{1}{2}} v_{n-1}(\xi)$$

$$\left(\xi - \frac{d}{d\xi}\right) v_n(\xi) = [2(n+1)]^{\frac{1}{2}} v_{n+1}(\xi)$$

which will play a role in the development of an operator approach to the SHO, given below.

1.4 Time-dependent states :

From the theory developed earlier we know that arbitrary time-dependent states can be built from the energy eigenstates :

$$\Psi(x,t) = \sum_{n=0}^{\infty} a_n \Psi_n(x,t)$$

$$= \sum_{n=0}^{\infty} a_n \psi_n(x) e^{-iE_n t/\hbar}$$

$$= e^{-i\omega t/2} \sum_{n=0}^{\infty} a_n \psi_n(x) e^{-in\omega t}$$

since $E_n = (n+\frac{1}{2})\hbar\omega$. We see that in general $|\Psi(x,t)|^2$ will depend on time, which is the sense in which the state is time-dependent.

To evaluate the coefficients a_n recall the general theory. A state $|\Psi\rangle$ may be expanded in a set of basis states:

$$|\Psi\rangle = \sum_\mu a_\mu |\mu\rangle$$

where the coefficients $a_\mu = \langle \mu | \Psi \rangle$.
For the case of energy eigenstates in the co-ordinate representation we ~~have~~ expect

$$\boxed{a_n = \int_{-\infty}^{+\infty} \Psi_n^* \Psi \, dx .}$$

It is easy to verify (using the orthonormality of the states ψ_n) that this equation is correct.

Alternatively, we can consider the "initial value problem": given $\Psi(x,0)$, how does the system subsequently evolve? First note that

$$\Psi(x,0) = \sum_{n=0}^{\infty} a_n \psi_n(x) .$$

Multiplying this by ψ_m & integrating gives

$$\int_{-\infty}^{+\infty} \Psi(x,0)\, \psi_m(x)\, dx = \sum_{n=0}^{\infty} a_n \int_{-\infty}^{+\infty} \psi_n(x)\psi_m(x)\, dx$$

$$= a_m$$

which allows calculation of the a_m.
With this knowledge, the future evolution of the system is simple: explicitly,

$$\Psi(x,t) = e^{\frac{-i\omega t}{2}} \sum_{n=0}^{\infty} \left(\int_{-\infty}^{+\infty} \Psi(x',0)\, \psi_n(x')\, dx' \right) \psi_n(x)\, e^{-in\omega t}.$$

NB. Determinism of the SE.

Note also that we require

$$\int_{-\infty}^{+\infty} |\Psi(x,0)|^2 dx = 1$$

i.e. $$\int_{-\infty}^{+\infty} \left(\sum_{n=0}^{\infty} a_n^* \psi_n \right) \left(\sum_{m=0}^{\infty} a_m \psi_m \right) dx = 1$$

i.e. $$\sum_{n=0}^{\infty} \sum_{m=0}^{\infty} a_n^* a_m \left(\int_{-\infty}^{+\infty} \psi_n \psi_m dx \right) = 1$$

or $$\boxed{\sum_{n=0}^{\infty} |a_n|^2 = 1}$$

which is the usual requirement on the coefficients in an expansion in eigenstates, since they represent probability amplitudes for being in a given eigenstate.

end of L6, 17/10

We can also explicitly calculate the expected energy of the system:

$$\langle E \rangle = \int_{-\infty}^{+\infty} \Psi^* \tilde{H} \Psi \, dx$$

where $\tilde{H} = \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2$. We have

$$\langle E \rangle = \int_{-\infty}^{+\infty} \left(\sum_{n=0}^{\infty} a_n^* \psi_n e^{in\omega t} \right) \tilde{H} \left(\sum_{m=0}^{\infty} a_m \psi_m e^{-im\omega t} \right)$$

$$= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} a_n^* a_m e^{-i(m-n)\omega t} \int_{-\infty}^{+\infty} \psi_n \tilde{H} \psi_m dx$$

$$= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} a_n^* a_m e^{-i(m-n)\omega t} \; E_m \delta_{m,n}$$

since $\tilde{H}\psi_m = E_m\psi_m$, & hence

$$\langle E \rangle = \sum_{n=0}^{\infty} E_n |a_n|^2.$$

DICE Q.

This is the expected result, since the a_n are probability amplitudes for being in the different energy eigenstates. A measurement of the energy of the system will return a particular eigenvalue E_n, with probability $|a_n|^2$.

The expectation value of energy is time-independent. However, the expectation value of position, is not:

$$\langle x \rangle = \int_{-\infty}^{+\infty} \Psi^* x \Psi \, dx$$

$$= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} a_n^* a_m e^{i(n-m)\omega t} \int_{-\infty}^{+\infty} \psi_n x \psi_m \, dx$$

i.e. $$\boxed{\langle x \rangle = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} a_n^* a_m e^{i(n-m)\omega t} x_{nm}}$$

where $$\boxed{x_{nm} = \int_{-\infty}^{+\infty} \psi_n x \psi_m \, dx.}$$ The elements x_{nm} form a matrix, which can be considered to be the matrix representation of the position operator in the co-ordinate representation. ~~More precisely, if we identify the spatial part of the energy eigenfunctions with~~ a state vectors $|n\rangle$:

See ERRATA

$$\psi_n(x) = \langle x | n \rangle$$

⊛ Note that the definition of matrix element that was previously given was the so-called Heisenberg picture, in which the matrix elements are time-dependent. The versions given here are the Schrodinger which are related as follows

$$\langle n|\overline{A}(t)|m\rangle = \langle n|A|m\rangle e^{i(E_n - E_m)t/\hbar}$$

See, e.g. pg. 361 of Merzbacher

More precisely we have

$$\langle n|\hat{x}|m\rangle = \int dx' \int dx \langle n|x\rangle\langle x|\hat{x}|x'\rangle\langle x'|m\rangle$$

↑ matrix element for $\hat{x}$

& $\langle x|\hat{x}|x'\rangle = \delta(x-x')\, x$

so $\langle n|\hat{x}|m\rangle = \int dx \langle n|x\rangle\, x\, \langle x|m\rangle$

so if we choose $\boxed{\langle x|m\rangle = \Psi_m(x,t)}$, we have

$$\langle n|\hat{x}|m\rangle = \int dx\, \Psi_n^*\, x\, \Psi_m$$

$$= e^{i(E_n-E_m)t/\hbar} \int_{-\infty}^{+\infty} \psi_n\, x\, \psi_m\, dx$$

$$= e^{i(E_n-E_m)t/\hbar}\, x_{nm}$$

& so x_{nm} differs from $\langle n|x|m\rangle$ only by complex exponential factors.

However, if we choose $\boxed{\langle x|m\rangle = \psi_m(x),}$ clearly we have

$$\langle n|\hat{x}|m\rangle = \int_{-\infty}^{+\infty} \psi_n\, x\, \psi_m\, dx$$

$$= x_{nm}.$$

WHY CAN WE "CHOOSE"?

$|n\rangle$ is defined by $\hat{H}|n\rangle = E_n|n\rangle$

$$\text{i.e.} \quad \langle x|\hat{H}|n\rangle = E_n\langle x|n\rangle$$

$$\text{i.e.} \quad \int dx' \langle x|\hat{H}|x'\rangle\langle x'|n\rangle = E_n\langle x|n\rangle$$

$$\text{i.e.} \quad \star \quad \langle x|\hat{H}|x'\rangle = \delta(x-x')\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V\right]$$

$$= \delta(x-x')\,\tilde{H}$$

$$\text{so} \qquad \tilde{H}\langle x|n\rangle = E_n\langle x|n\rangle$$

which is satisfied by <u>both</u> ψ_n & E_n

With the choice $\langle x|n\rangle = \psi_n(x)$ the matrix elements (& basis vectors $|n\rangle$) have no time dependence. This is the "Schrodinger picture" of time development. (the other choice is the "Heisenberg picture")

So in the following we adopt the S.P. ~~them~~ of write

$$\boxed{\langle n|\hat{x}|m\rangle = x_{nm}\,,}$$

which accords with Jim's notation (*) ⇐

To evaluate the x_{nm}, first re-write the associated integral in terms of $\xi = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}} x$:

$$x_{nm} = \left(\frac{\hbar}{m\omega}\right)^{\frac{1}{2}} \int_{-\infty}^{+\infty} d\xi \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}} v_n(\xi) v_m(\xi) \left(\frac{\hbar}{m\omega}\right)^{\frac{1}{2}} \xi$$

$\psi_n(x) = \left|\frac{d\xi}{dx}\right|^{\frac{1}{2}} v_n(\xi)$

$$= \left(\frac{\hbar}{m\omega}\right)^{\frac{1}{2}} \int_{-\infty}^{+\infty} d\xi\, v_n(\xi) v_m(\xi)\, \xi$$

Recall the earlier relationships:

$$\left(\xi + \frac{d}{d\xi}\right) v_n = (2n)^{\frac{1}{2}} v_{n-1}$$

$$\left(\xi - \frac{d}{d\xi}\right) v_n = [2(n+1)]^{\frac{1}{2}} v_{n+1}\,.$$

Adding these gives

$$\xi v_n = \tfrac{1}{2}\left[(2n)^{\frac{1}{2}} v_{n-1} + \{2(n+1)\}^{\frac{1}{2}} v_{n+1}\right]$$

& hence

$$x_{nm} = \tfrac{1}{2}\left(\frac{\hbar}{m\omega}\right)^{\frac{1}{2}}\Big[(2n)^{\frac{1}{2}} \int_{-\infty}^{+\infty} v_{n-1} v_m\, d\xi + \{2(n+1)\}^{\frac{1}{2}} \int_{-\infty}^{+\infty} v_{n+1} v_m\, d\xi\Big]$$

i.e. $$\boxed{x_{nm} = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}\left[n^{\frac{1}{2}}\delta_{n-1,m} + (n+1)^{\frac{1}{2}}\delta_{n+1,m}\right]}$$

end of L87, 18/10.

or in matrix notation: ⟶ m

$$[x_{nm}] = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}} \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix}.$$

or $[\langle n|\hat{x}|m\rangle]$; ↓ n

Similarly we can use our co-ordinate representation to establish the matrix elements of the operator $\hat{p}$ (exercise):

$$\left[\langle n|\hat{p}|m\rangle\right] = i\left(\frac{m\hbar\omega}{2}\right)^{\frac{1}{2}} \begin{pmatrix} 0 & -\sqrt{1} & 0 & 0 & \cdots \\ \sqrt{1} & 0 & -\sqrt{2} & 0 & \cdots \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix}$$

"the matrix representing the operator"

Given that the expectation value for position is time-dependent, how does it evolve?

Recall

$$\langle x\rangle = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} a_n^* a_m e^{i(n-m)\omega t} x_{nm}$$

$$\text{so } \frac{d^2\langle x\rangle}{dt^2} = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} a_n^* a_m \left[-(n-m)^2\omega^2\right] e^{i(n-m)\omega t} \cdot x_{nm}$$

Now the $x_{nm} = 0$ except if $n = m \pm 1$, so the factor $(n-m)^2$ is unity, & we have

Q.

$$\boxed{\frac{d^2\langle x\rangle}{dt^2} = -\omega^2\langle x\rangle}$$

which is the equation of motion for the classical SHO! Hence the expectation value for position oscillates like the classical particle. This is a special case of Ehrenfest's theorem, which states that expectation values of QM operators obey laws similar to those of classical physics.

1.5 Creation & annihilation operators :

Dirac arrived at a treatment of the SHO that avoids wavefunctions entirely. He began with the Hamiltonian $\hat{H}$ expressed in terms of the position & momentum operators:

$$\hat{H} = \hat{P}^2/2m + \tfrac{1}{2}m\omega^2\hat{X}^2.$$

He defined two new operators:

$$\hat{a} = \frac{1}{(2\hbar m\omega)^{\frac{1}{2}}}(m\omega\hat{x} + i\hat{p})$$

$$\hat{a}^\dagger = \frac{1}{(2\hbar m\omega)^{\frac{1}{2}}}(m\omega\hat{x} - i\hat{p})$$

← dagger, not plus

In the co-ordinate representation

$$\hat{a} \to \tilde{a} = \frac{1}{\sqrt{2}}\left(\xi + \frac{d}{d\xi}\right)$$

$$\hat{a}^\dagger \to \tilde{a}^\dagger = \frac{1}{\sqrt{2}}\left(\xi - \frac{d}{d\xi}\right).$$

Recalling the recursion relations

$$\left(\xi + \frac{d}{d\xi}\right)v_n = (2n)^{\frac{1}{2}}v_{n-1}$$

$$\left(\xi - \frac{d}{d\xi}\right)v_n = [2(n+1)]^{\frac{1}{2}}v_{n+1}$$

we have

$$\tilde{a}\,v_n = n^{\frac{1}{2}}v_{n-1}$$

$$\tilde{a}^\dagger v_n = (n+1)^{\frac{1}{2}}v_{n+1}$$

The operator $\tilde{a}$ is the "annihilation" operator. It lowers the oscillator by one energy level, or reduces the number of quanta by one. The operator $\tilde{a}^\dagger$ is the "creation" operator, which raises the number of quanta by one. These operators are called variously in the literature

raising/lowering operators, step-up/step-down operators, & ladder operators.

Although we have worked in the co-ordinate representation, it is clear that there should be more general representations of these operators, & so we ~~expect~~ write

$$\hat{a}|n\rangle = n^{\frac{1}{2}}|n-1\rangle$$
$$\& \quad \hat{a}^\dagger|n\rangle = (n+1)^{\frac{1}{2}}|n+1\rangle$$

where $|n\rangle$ represents the energy eigenstate with n quanta. It follows that the matrix representation of these operators is

$$\langle n|\hat{a}|m\rangle = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix}$$

$\langle n|\hat{a}|m\rangle$
$= m^{\frac{1}{2}}\langle n|m-1\rangle$
$= m^{\frac{1}{2}}\delta_{n,m-1}$

$$\& \quad \langle n|\hat{a}^\dagger|m\rangle = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix}$$

The creation operator can be used to construct the higher states by repeated operation on the ground state $|0\rangle$:

$$|n\rangle = \frac{(\hat{a}^+)^n}{(n!)^{\frac{1}{2}}} |0\rangle$$

In addition we require that the ground state gives zero when operated on by the annihilation operator:

$$\hat{a}|0\rangle = 0$$

$$\text{or } \frac{1}{\sqrt{2}}\left(\xi + \frac{d}{d\xi}\right) v_0(\xi) = 0 ,$$

in the co-ordinate representation. Integrating the last equation gives a very quick way to obtain the explicit wavefunctions:

$$\frac{dv_0}{d\xi} + \xi v_0 = 0$$

$$\int \frac{dv_0}{v_0} = -\int \xi \, d\xi$$

$$\ln v_0 = -\frac{1}{2}\xi^2 + \text{const.}$$

$$\text{i.e. } v_0 = A e^{-\frac{1}{2}\xi^2}$$

* normalisation $\Rightarrow$ $A = \pi^{-\frac{1}{4}}$

1.6 A wavefunction-free approach to the SHO

Although we have arrived at the wavefunctions, the properties of the SHO can be determined again without introducing

at all
wavefunctions, by considering the properties of the operators $\hat{a}$ & $\hat{a}^\dagger$.

restate def'n: ?

First, consider

$$\hat{a}\hat{a}^\dagger = (2\hbar m\omega)^{-1}(m\omega\hat{x} + i\hat{p})(m\omega\hat{x} - i\hat{p})$$

$$= (2\hbar m\omega)^{-1}(m^2\omega^2\hat{x}^2 + \hat{p}^2 - im\omega[\hat{x},\hat{p}])$$

$$= (2\hbar m\omega)^{-1}(m^2\omega^2\hat{x}^2 + \hat{p}^2 + m\omega\hbar)$$

using the basic commutation relation $[\hat{x},\hat{p}] = i\hbar$.

Hence $$\hat{a}\hat{a}^\dagger = \frac{1}{2} + \frac{1}{\hbar\omega}\left(\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2\right)$$

$$= \frac{1}{2} + \frac{\hat{H}}{\hbar\omega}$$

Similarly $$\hat{a}^\dagger\hat{a} = \frac{\hat{H}}{\hbar\omega} - \frac{1}{2}$$

Next
$\hat{a}\hat{a}^\dagger$ — end of L8, @ 20/10

Using these results we can establish the basic commutation relations for the creation & annihilation operators:

$$[\hat{a},\hat{a}^\dagger] = 1 \quad [\hat{a},\hat{H}] = \hbar\omega\hat{a}, \quad [\hat{a}^\dagger,\hat{H}] = -\hbar\omega\hat{a}^\dagger$$

Exercise: prove these.

Now consider a system with energy E, so that $\hat{H}|E\rangle = E|E\rangle$. Then

$$\hat{H}\hat{a}|E\rangle = \{\hat{a}\hat{H} - [\hat{a},\hat{H}]\}|E\rangle$$

$$= \{\hat{a}\hat{H} - \hbar\omega\hat{a}\}|E\rangle$$

$$= (E - \hbar\omega)\hat{a}|E\rangle \qquad (1)$$

& $$\hat{H}\hat{a}^\dagger|E\rangle = \{\hat{a}^\dagger\hat{H} - [\hat{a}^\dagger,\hat{H}]\}|E\rangle$$

$$= \{\hat{a}^\dagger\hat{H} + \hbar\omega\hat{a}^\dagger\}|E\rangle$$

$$= (E + \hbar\omega)\hat{a}^\dagger|E\rangle \qquad (2)$$

Equation (1) says that the state $\hat{a}|E\rangle$ is also an energy eigenstate, with eigenvalue (energy) $E - \hbar\omega$. Similarly (2) says $\hat{a}^\dagger|E\rangle$ is an eigenstate, with energy $E + \hbar\omega$. Hence we can construct states with energy $E \pm \hbar\omega$, $E \pm 2\hbar\omega$, & so on. However, the Hamiltonian is non-negative (it is a sum of squares) & so its eigenvalues must be positive. Hence there must be a lowest state $|E_0\rangle$, with $\hat{H}|E_0\rangle = E_0|E_0\rangle$. Operating on this state with the annihilation operator must give zero, i.e. $\hat{a}|E_0\rangle = 0$.

From the expression above for the Hamiltonian we have

$$\hat{H}|E_0\rangle = \hbar\omega(\hat{a}^\dagger\hat{a} + \tfrac{1}{2})|E_0\rangle$$

$$= \tfrac{1}{2}\hbar\omega|E_0\rangle,$$

since $\hat{a}|E_0\rangle = 0$. Hence we identify the eigenvalue of the lowest state: $E_0 = \frac{1}{2}\hbar\omega$. By acting on that state with the creation operator it follows that the energy eigenvalues are $E_n = (n+\frac{1}{2})\hbar\omega$.* Note that this entire argument relies only on the assumed forms for $\hat{a}$ & $\hat{a}^\dagger$ & the basic commutator relation $[\hat{x}, \hat{p}] = i\hbar$. Hence we have arrived at the correct eigenvalues without recourse to the wavefunctions, or the co-ord. representation.

Notice finally that

$$\hat{H}|E_n\rangle = \hbar\omega(\hat{a}^\dagger a + \tfrac{1}{2})|E_n\rangle$$

$$= E_n|E_n\rangle$$

$$= (n+\tfrac{1}{2})\hbar\omega|E_n\rangle$$

which implies $\hat{a}^\dagger\hat{a} = n$. Thus $\hat{a}^\dagger\hat{a}$ is often called the number operator: it yields the number of quanta in a state.

---

* The states $|E_n\rangle$ were labelled $|n\rangle$ earlier.

3. ANGULAR MOMENTUM :

The SHO is an example of a 1-D QM system. Particle motion in 3-D introduces the important idea of orbital angular momentum. Like every physical observable, in QM orbital angular momentum is represented by an operator. We know from classical physics that orbital AM is especially useful in the solution of problems involving a central force, & we will see that this is also the case in QM.

There is also another kind of AM, that is intrinsic to a particle – spin. Jim has discussed in some detail how the spin of an electron can be determined via the Stern-Gerlach experiment.

Before discussing orbital AM & then spin in QM, we begin with a review of the ideas of measurement & commutators.

3.1 Measurement & commutators :

First recall that operators corresponding to observables that are simultaneously measurable to arbitrary precision ("compatible") commute.

For example, the x & y co-ordinates of

a particle are simultaneously measurable to arbitrary precision, &

$$[\hat{x}, \hat{y}] = 0.$$

Operators corresponding to observables that satisfy an uncertainty relation do not commute. For example, $[\hat{x}, \hat{p}_x] = i\hbar$, which corresponds to the uncertainty relation

$$\Delta x \, \Delta p_x \geq \frac{\hbar}{2}$$

The commutators of arbitrary operators satisfy the following relations, which will be handy in our treatment of AM:

(C1) $[\hat{A}, \hat{A}] = 0$

(C2) $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$

(C3) $[\hat{A}+\hat{B}, \hat{C}] = [\hat{A}, \hat{C}] + [\hat{B}, \hat{C}]$

(C4) $[\hat{A}, \hat{B}+\hat{C}] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}]$

(C5) $[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$

(C6) $[\hat{A}\hat{B}, \hat{C}] = [\hat{A}, \hat{C}]\hat{B} + \hat{A}[\hat{B}, \hat{C}]$

Exercise: check these!

Mathematically, if two observables are simultaneously measurable to arbitrary accuracy, then there must be a set of simultaneous

Finally, recall that operators corresponding to physical observables are Hermitian, i.e. the adjoint, or Hermitian conjugate of the operator is the original operator:

$$\hat{Q}^\dagger \equiv \hat{Q}$$

(c1) $[\hat{A}, \hat{A}] = 0$

(c2) $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$

(c3) $[\hat{C}, \hat{B}] + [\hat{C}, \hat{A}] = [\hat{C}, \hat{B}+\hat{A}]$

(c4) $[\hat{C}, \hat{A}] + [\hat{B}, \hat{A}] = [\hat{C}+\hat{B}, \hat{A}]$

(c5) $[\hat{C}, \hat{A}]\hat{B} + \hat{C}[\hat{B}, \hat{A}] = [\hat{C}\hat{B}, \hat{A}]$

(c6) $[\hat{C}, \hat{B}]\hat{A} + \hat{B}[\hat{C}, \hat{A}] = [\hat{C}, \hat{B}\hat{A}]$

Exercise: check them!

complete
eigenstates for the two operators representing the observables. It is easy to show that if there are common eigenstates, the operators commute: suppose we have $|A_i B_j\rangle$ st

$$\hat{A}\,|A_i B_j\rangle = A_i\,|A_i B_j\rangle$$

& $$\hat{B}\,|A_i B_j\rangle = B_j\,|A_i B_j\rangle,$$

for all eigenvalues A_i, B_j. Then

$$\hat{A}\hat{B}\,|A_i B_j\rangle = A_i B_j\,|A_i B_j\rangle$$
$$= B_j A_i\,|A_i B_j\rangle$$
$$= \hat{B}\hat{A}\,|A_i B_j\rangle$$

i.e. $$(\hat{A}\hat{B} - \hat{B}\hat{A})\,|A_i B_j\rangle = 0$$

& since this must hold for all the eigenstates, we have

extra ← (*) $$\hat{A}\hat{B} = \hat{B}\hat{A} \quad \text{or} \quad [\hat{A}, \hat{B}] = 0.$$ end of L9, 23/10

3.2 Commutation relations for orbital angular momentum

The orbital AM of a classical particle is given by $\underset{\sim}{L} = \underset{\sim}{x} \times \underset{\sim}{p}$. In QM the orbital angular momentum operator is

$$\boxed{\hat{\underset{\sim}{L}} = \hat{\underset{\sim}{x}} \times \hat{\underset{\sim}{p}}}$$ ORBITAL AM

The components of the operator are

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y$$
$$\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z$$
$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$$

We can establish sets of commutation relations for the components of AM. For example, for $\hat{L}_x$ we have (exercise)

$$[\hat{L}_x, \hat{x}] = 0\,, \quad [\hat{L}_x, \hat{y}] = -i\hbar\hat{z}\,, \quad [\hat{L}_x, \hat{z}] = -i\hbar\hat{y}$$
$$[\hat{L}_x, \hat{p}_x] = 0\,, \quad [\hat{L}_x, \hat{p}_y] = i\hbar\hat{p}_z\,, \quad [\hat{L}_x, \hat{p}_z] = -i\hbar\hat{p}_y.$$

As an example of how these are obtained, consider the first:

$$[\hat{L}_x, \hat{x}] = [\hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \hat{x}]$$
$$= [\hat{y}\hat{p}_z, \hat{x}] - [\hat{z}\hat{p}_y, \hat{x}] \quad \text{, by (C3)}$$
$$= [\hat{y}, \hat{x}]\hat{p}_z + \hat{y}[\hat{p}_z, \hat{x}] - [\hat{z}, \hat{x}]\hat{p}_y - \hat{z}[\hat{p}_y, \hat{x}]\,,$$
using (C6)
$$= 0$$

Using these commutation relations & the corresponding ones for $\hat{L}_y$ & $\hat{L}_z$ it is straightforward to establish the commutation relations among the components of the AM operator:

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$$
$$[\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x$$
$$[\hat{L}_z, \hat{L}_x] = i\hbar \hat{L}_y$$

ORBITAL AM COMMUTATION REL'NS

cyclical : always order

As an example, we will establish the 1st of these:

$$[\hat{L}_x, \hat{L}_y] = [\hat{L}_x, \hat{z}\hat{p}_x - \hat{x}\hat{p}_z]$$
$$= [\hat{L}_x, \hat{z}\hat{p}_x] - [\hat{L}_x, \hat{x}\hat{p}_z]$$
$$= [\hat{L}_x, \hat{z}]\hat{p}_x + \hat{z}[\hat{L}_x, \hat{p}_x] - [\hat{L}_x, \hat{x}]\hat{p}_z - \hat{x}[\hat{L}_x, \hat{p}_z] \quad \text{by (C5)}$$
$$= -i\hbar \hat{y}\hat{p}_x + 0 - 0 + i\hbar \hat{x}\hat{p}_y$$
$$= i\hbar(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x) = i\hbar \hat{L}_z$$

The 3 commutation relations for the components of the orbital AM operator may be summarised by the vector r'ship

$$\hat{\underset{\sim}{L}} \times \hat{\underset{\sim}{L}} = i\hbar \hat{\underset{\sim}{L}}$$

exercise: check this

(NB. it is clear from this r'ship that $\hat{\underset{\sim}{L}}$ must be an operator: if it were just a vector then this r'ship would imply $\underset{\sim}{L} = 0$).

The commutation relations for the components of the orbital AM operator do not commute, so two components of the orbital AM cannot be simultaneously measured with arbitrary accuracy.

The operator representing the square of the obital AM is

$$\boxed{\hat{\underset{\sim}{L}}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2}$$

We can rewrite this operator in terms of the position & momentum operators as follows.

$$\hat{\underset{\sim}{L}}^2 = (\hat{\underset{\sim}{x}} \times \hat{\underset{\sim}{p}}) \cdot (\hat{\underset{\sim}{x}} \times \hat{\underset{\sim}{p}})$$

$$= (\hat{\underset{\sim}{x}} \cdot \hat{\underset{\sim}{x}})(\hat{\underset{\sim}{p}} \cdot \hat{\underset{\sim}{p}}) - (\hat{\underset{\sim}{x}} \cdot \hat{\underset{\sim}{p}})(\hat{\underset{\sim}{p}} \cdot \hat{\underset{\sim}{x}})$$

[using the vector ID $(\underset{\sim}{A} \times \underset{\sim}{B}) \cdot (\underset{\sim}{C} \times \underset{\sim}{D}) = (\underset{\sim}{A} \cdot \underset{\sim}{C})(\underset{\sim}{B} \cdot \underset{\sim}{D}) - (\underset{\sim}{A} \cdot \underset{\sim}{D})(\underset{\sim}{B} \cdot \underset{\sim}{C})$]

Hence $\hat{\underset{\sim}{L}}^2 = \hat{\underset{\sim}{x}}^2 \hat{\underset{\sim}{p}}^2 - \hat{\underset{\sim}{x}} \cdot \hat{\underset{\sim}{p}} \left(- [\hat{\underset{\sim}{x}}, \hat{\underset{\sim}{p}}] + \hat{\underset{\sim}{x}} \cdot \hat{\underset{\sim}{p}} \right)$

$$= \hat{\underset{\sim}{x}}^2 \hat{\underset{\sim}{p}}^2 - \hat{\underset{\sim}{x}} \cdot \hat{\underset{\sim}{p}} \left(-i\hbar + \hat{\underset{\sim}{x}} \cdot \hat{\underset{\sim}{p}} \right)$$

so $$\boxed{\hat{\underset{\sim}{L}}^2 = \hat{\underset{\sim}{x}}^2 \hat{\underset{\sim}{p}}^2 - (\hat{\underset{\sim}{x}} \cdot \hat{\underset{\sim}{p}})^2 + i\hbar \hat{\underset{\sim}{x}} \cdot \hat{\underset{\sim}{p}}}$$

3.3 Arbitrary AM

Although we have considered only orbital AM, any vector operator $\hat{\underset{\sim}{J}}$ that satisfies the commutation relations

$$[\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z$$
$$[\hat{J}_y, \hat{J}_z] = i\hbar \hat{J}_x$$
$$[\hat{J}_z, \hat{J}_x] = i\hbar \hat{J}_y$$

ARBITRARY AM COMMUTATION REL'NS

(or more succinctly, $\hat{\underset{\sim}{J}} \times \hat{\underset{\sim}{J}} = i\hbar \hat{\underset{\sim}{J}}$) is called an angular momentum operator in QM. (end of Lec 29/10) This includes orbital AM, which we have already considered, & spin AM. [NB however: only orbital AM is given by $\hat{\underset{\sim}{x}} \times \hat{\underset{\sim}{p}}$.] when specifically referring to orbital, often written $\hat{\underset{\sim}{L}}$: spin $\hat{\underset{\sim}{S}}$

Next note that, according to the comm. relations

$$[\hat{\underset{\sim}{J}}^2, \hat{J}_x] = [\hat{J}_x^2, \hat{J}_x] + [\hat{J}_y^2, \hat{J}_x] + [\hat{J}_z^2, \hat{J}_x]$$

$$= 0 + [\hat{J}_y, \hat{J}_x]\hat{J}_y + \hat{J}_y[\hat{J}_y, \hat{J}_x] + [\hat{J}_z, \hat{J}_x]\hat{J}_z + \hat{J}_z[\hat{J}_z, \hat{J}_x]$$

$$= -i\hbar \hat{J}_z \hat{J}_y - i\hbar \hat{J}_y \hat{J}_z + i\hbar \hat{J}_y \hat{J}_z + i\hbar \hat{J}_z \hat{J}_y$$

$$= 0$$

& similarly $[\hat{\underset{\sim}{J}}^2, \hat{J}_y] = [\hat{\underset{\sim}{J}}^2, \hat{J}_z] = 0$, so we have

$$\boxed{[\hat{\underset{\sim}{J}}^2, \hat{\underset{\sim}{J}}] = 0}$$

Hence $\hat{\underset{\sim}{J}}^2$ & any of the components of $\hat{\underset{\sim}{J}}$ are compatible. Usually $\hat{\underset{\sim}{J}}^2$ & $\hat{J}_z$ are taken as the commuting operators used to describe an arbitrary AM.* NB. Arbitrary! Because the operators $\hat{\underset{\sim}{J}}^2$ & $\hat{J}_z$ are compatible, there exist simultaneous eigenstates $|J'^2 J_z'\rangle$, with eigenvalues J'^2 & J_z' respectively:

$$\boxed{\hat{J}_z |J'^2 J_z'\rangle = J_z' |J'^2 J_z'\rangle}$$

$$\& \quad \boxed{\hat{\underset{\sim}{J}}^2 |J'^2 J_z'\rangle = J'^2 |J'^2 J_z'\rangle}$$

Next we introduce the operators

$$\boxed{\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y,}$$

which we will see play the role of raising & lowering operators for the eigenstates of $\hat{J}_z$. First note that

$$\begin{aligned}
[\hat{J}_\pm, \hat{J}_z] &= [\hat{J}_x \pm i\hat{J}_y, \hat{J}_z] \\
&= [\hat{J}_x, \hat{J}_z] \pm i[\hat{J}_y, \hat{J}_z] \\
&= -i\hbar\hat{J}_y \pm i.\, i\hbar J_x \\
&= -i\hbar\hat{J}_y \mp \hbar\hat{J}_x \\
&= \mp\hbar\hat{J}_\pm
\end{aligned}$$

i.e. $$\boxed{[\hat{J}_\pm, \hat{J}_z] = \mp\hbar\hat{J}_\pm}$$

Next consider the action of $\hat{J}_z$ on $\hat{J}_\pm|J'^2 J_z'\rangle$:

$$\hat{J}_z\left(\hat{J}_\pm|J'^2 J_z'\rangle\right) = \left(\hat{J}_\pm\hat{J}_z - [\hat{J}_\pm, J_z]\right)|J'^2 J_z'\rangle$$
$$= \left(\hat{J}_\pm J_z' \pm \hbar\hat{J}_\pm\right)|J'^2 J_z'\rangle$$
$$= \left(J_z' \pm \hbar\right)\hat{J}_\pm|J'^2 J_z'\rangle$$

which establishes that $\hat{J}_\pm|J'^2 J_z'\rangle$ are eigenstates of $\hat{J}_z$, with eigenvalues $J_z' \pm \hbar$. The states $\hat{J}_\pm|J'^2 J_z'\rangle$ are not necessarily normalized. Consider the inner product

$$\left(\langle J'^2 J_z'|\hat{J}_\pm^\dagger\right)\left(\hat{J}_\pm|J'^2 J_z'\rangle\right) = \langle J'^2 J_z'|\hat{J}_\mp\hat{J}_\pm|J'^2 J_z'\rangle,$$

since $\hat{J}_\pm^\dagger = (\hat{J}_x \pm i\hat{J}_y)^\dagger = (\hat{J}_x^\dagger \mp i\hat{J}_y^\dagger) = (\hat{J}_x \mp i\hat{J}_y)$
$= \hat{J}_\mp$

since $\hat{J}_x$ & $\hat{J}_y$ are Hermitian. Next consider the product $\hat{J}_\mp\hat{J}_\pm$:

$$\hat{J}_\mp\hat{J}_\pm = (\hat{J}_x \mp i\hat{J}_y)(\hat{J}_x \pm i\hat{J}_y)$$
$$= \hat{J}_x^2 + \hat{J}_y^2 \pm i[\hat{J}_x, \hat{J}_y]$$
$$= \hat{J}_x^2 + \hat{J}_y^2 \mp \hbar\hat{J}_z = \hat{J}^2 - \hat{J}_z^2 \mp \hbar\hat{J}_z$$

Hence we have rewrite in a box!

$$\boxed{\left(\langle J'^2 J_z'|\hat{J}_\pm^\dagger\right)\left(\hat{J}_\pm|J'^2 J_z'\rangle\right) = \left(J'^2 - J_z'^2 \mp \hbar J_z'\right)\langle J'^2 J_z'|J'^2 J_z'\rangle}$$

Consider the factors

$$f(J_z') = J'^2 - J_z'^2 - \hbar J_z'$$

& $$g(J_z') = J'^2 - J_z'^2 + \hbar J_z'$$

Both factors must be positive. The term J'^2 represents the square of the total AM, & can be considered to be constant for a given system. For some large (positive) value of J_z', $f(J_z') = 0$. This imposes an upper limit on J_z':

$$(J_z')^2_{max} + \hbar (J_z')_{max} = J'^2 \qquad (1)$$

Similarly, for some large negative value of J_z', $g(J_z') = 0$. This imposes a lower limit on J_z':

$$(J_z')^2_{min} - \hbar (J_z')_{min} = J'^2 \qquad (2)$$

Note that these results will ensure that operating on the highest state with $\hat{J}_+$ gives zero, & operating on the lowest state with $\hat{J}_-$ gives zero.

Next assume $\boxed{(J_z')_{max} = \hbar j}$ (j is arbitrary at this point). Then (1) $\Rightarrow$

$$\hbar^2 j^2 + \hbar^2 j = J'^2$$

$$\text{i.e. } \boxed{J'^2 = \hbar^2 j(j+1)}$$

end of L.11
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& then (2) $\Rightarrow$

$$(J_z')^2_{min} - \hbar (J_z')_{min} = \hbar^2 j(j+1)$$

$$\text{i.e. } (J_z')^2_{min} - \hbar (J_z')_{min} - \hbar^2 j(j+1) = 0$$

$$\text{i.e. } (J_z')_{min} = \frac{\hbar \pm \left[\hbar^2 + 4\hbar^2 j(j+1)\right]^{\frac{1}{2}}}{2}$$

$$= \left(\hbar \pm \hbar \left[1 + 4j^2 + 4j\right]^{\frac{1}{2}}\right)/2$$

i.e. $(J_z')_{min} = \dfrac{\hbar \pm \hbar(2j+1)}{2}$

$= \hbar(j+1), -\hbar j$

& since we require $(J_z')_{min} < (J_z')_{max} = \hbar j$, we take

$$\boxed{(J_z')_{min} = -\hbar j.}$$

Using the raising operator to get from $|J'^2 (J_z')_{min}\rangle$ to $|J'^2 (J_z')_{max}\rangle$ implies

$$(J_z')_{max} - (J_z')_{min} = \hbar \times \text{integer}$$

(since $\hat{J}_\pm |J'^2 J_z'\rangle$ are eigenstates of $\hat{J}_z$ with eigenvalues $J_z' \pm \hbar$). But we have established

$$(J_z')_{max} - (J_z')_{min} = 2\hbar j$$

& so we conclude that

$$\boxed{2j \text{ is an integer}}$$

We have that $(J_z')_{min} = -\hbar j$, & J_z' increases in steps of $\hbar$. Hence

$$\boxed{J_z' = m\hbar, \quad m = -j, (j-1), \cdots, (j-1), j}$$

where $2j$ is an integer. It is convenient to relabel the eigenstates in terms of m & j, viz.

$$\boxed{|J'^2 J_z'\rangle \rightarrow |jm\rangle}$$

(when referring to orbital, see $|\ell m\rangle$)

To summarise, we have established the following important result for an arbitrary AM in QM, represented by the operator $\hat{\underset{\sim}{J}}$:

1. The operator $\hat{\underset{\sim}{J}}^2$ has eigenvalues

$$\underset{\sim}{J}'^2 = \hbar^2 j(j+1)$$

where $2j$ is an integer

2. The compatible observable $\hat{J}_z$ has eigenvalues

$$J_z' = \hbar m, \text{ where}$$

$$m = -j, -(j-1), \ldots, (j-1), j$$

- so for every j there are $2j+1$ eigenstates for $\hat{J}_z$

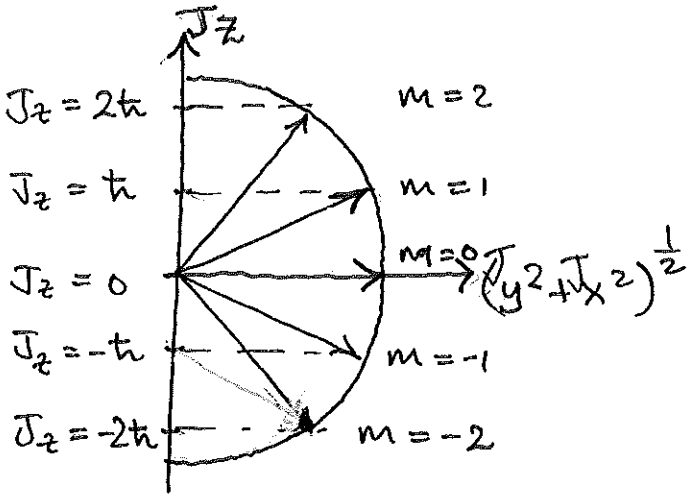
Physically the eigenvalue $\underset{\sim}{J}'^2$ corresponds to the total AM of the state. The eigenvalues of $\hat{J}_z$ represent the projection of the AM vector onto the z axis. However, the x & y components of the angular momentum vector are not well defined, if J_z' is known, since $\hat{J}_x$ & $\hat{J}_z$ & $\hat{J}_y$ & $\hat{J}_z$ do not commute. Hence we cannot think of the AM vector as having a definite direction in space: instead we think of the vector as being distributed over all directions in the x-y plane at once.

However, they must also take the values $m = -j, -(j-1), \ldots, (j-1), j$ but the exact value returned is only prob.

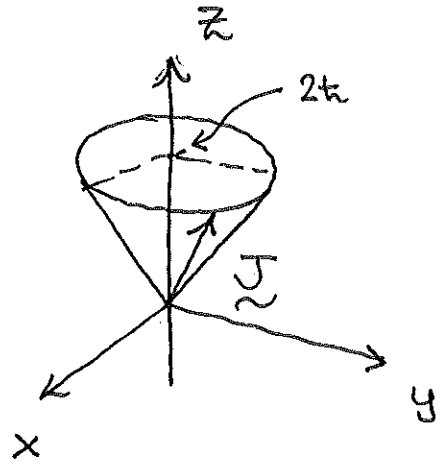
* Note that for a system in a state, $\psi = Y_{2,m}$, a measurement of any component of $\vec{J}$, i.e. J_x or J_y results in one of the values $m\hbar$ with, $m = -2, -1, 0, 1, 2$. We have chosen to concentrate on J_z.

The AM vector then defines a cone.

e.g. for $j = 2$



possible orientations



$m = 2$ state

$*$ Note finally that the action of the raising & lowering operators can now be determined explicitly. We have

$$\hat{J}_+ |j\,m\rangle = c_+ |j\,m+1\rangle$$

& $$\hat{J}_- |j\,m\rangle = c_- |j\,m-1\rangle$$

where $c_\pm$ can be determined from

$$\langle j\,m | J_\pm^\dagger J_\pm | j\,m\rangle = (J^2 - J_z^2 \mp \hbar J_z) \langle j\,m | j\,m\rangle$$

$$= c_\pm^2 .$$

Assuming the states $|j\,m\rangle$ are normalised, we have

$$c_\pm^* = [J^2 - J_z^2 \mp \hbar J_z]^{\frac{1}{2}}$$

$$= [\hbar^2 j(j+1) - \hbar^2 m^2 \mp \hbar^2 m]^{\frac{1}{2}}$$

$$= \hbar [(j \mp m)(j \pm m + 1)]^{\frac{1}{2}}$$

where the last step is left as an exercise.

Hence we have

$$\hat{J}_+ |jm\rangle = \hbar \sqrt{(j-m)(j+m+1)}\, |j\, m+1\rangle$$

&

$$\hat{J}_- |jm\rangle = \hbar \sqrt{(j+m)(j-m+1)}\, |j\, m-1\rangle$$

So far we have not discussed the possible values of j, beyond establishing that $2j$ must be an integer. We shall see later that for orbital angular momentum, j is an integer. Half integral values of j occur for the spin of various particles. For example, Jim has discussed the spin of the electron (for which $j = \frac{1}{2}$) in some detail.

The results we have presented are completely general, & independent of any particular representation. We now discuss two representations of the AM operators & eigenstates: the matrix representation, & the wavefunction representation.

end of L12

3.4 Matrix representation of AM:

For the operator $\underset{\sim}{\hat{J}}^2$, the elements of the matrix are

$$\langle jm | \underset{\sim}{\hat{J}}^2 | j' m' \rangle,$$

where the values of j & m are ordered in some way. For each j there are $(2j+1)$ values of m. We can construct

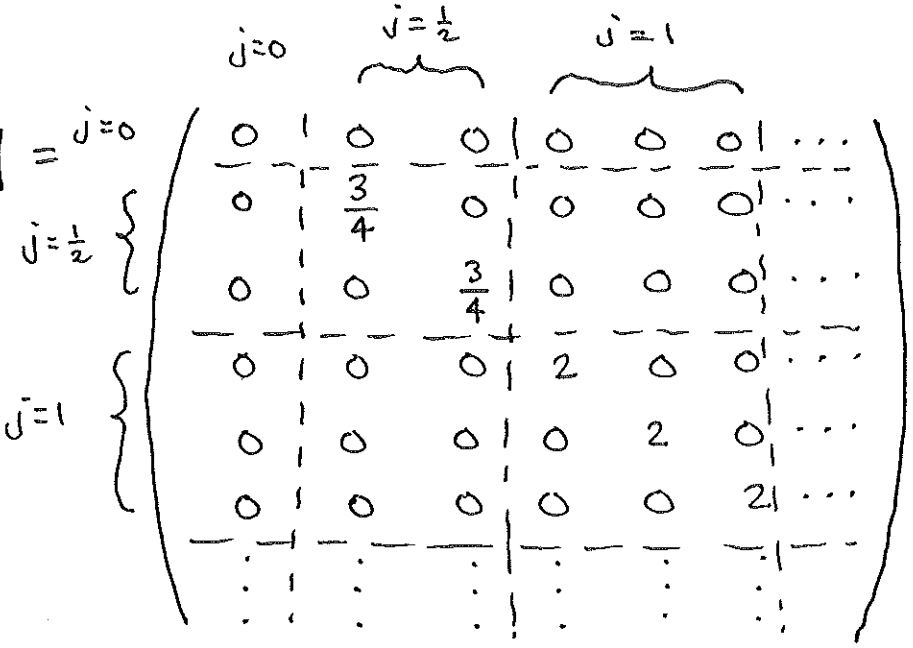
a matrix representation for all possible values of j by adopting the ordering

$$|j=0, m=0\rangle,\ |j=\tfrac{1}{2}, m=\tfrac{1}{2}\rangle,\ |j=\tfrac{1}{2}, m=-\tfrac{1}{2}\rangle,$$

$$|j=1, m=1\rangle,\ |j=1, m=0\rangle,\ |j=1, m=-1\rangle,\ \ldots$$

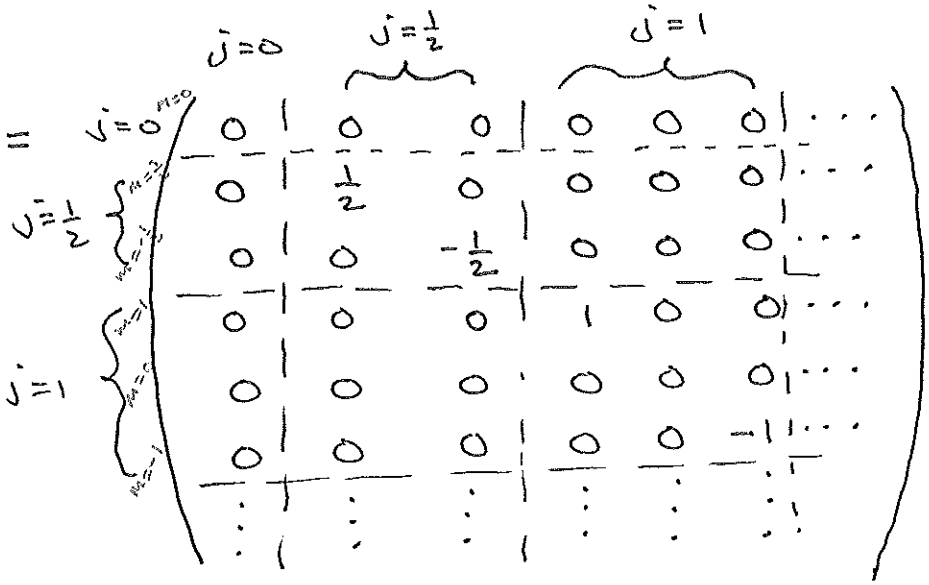
i.e. by ordering first by the j value (in increasing order) & then by the m value (in decreasing order). Recalling that the eigenvalues of $\hat{\underset{\sim}{J}}^2$ are $\hbar^2 j(j+1)$, we have

$$\frac{1}{\hbar^2}\left[\langle jm|\hat{\underset{\sim}{J}}^2|j'm'\rangle\right] =$$



For $\hat{J}_z$, the eigenvalues are $\hbar m$, so

$$\frac{1}{\hbar}\left[\langle jm|\hat{J}_z|j'm'\rangle\right] =$$



The simultaneous eigenstates for these operators are represented by infinite column vectors with a 1 at the appropriate entry, and zeroes for all other entries,

$$\text{i.e. } |0\,0\rangle \to \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \quad |\tfrac{1}{2},\tfrac{1}{2}\rangle \to \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}, \quad |\tfrac{1}{2},-\tfrac{1}{2}\rangle \to \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix}, \ldots$$

It is easy to see why this is so by considering one example: for instance the eigenvalue equation

$$\hat{J}_z |\tfrac{1}{2},\tfrac{1}{2}\rangle = \tfrac{1}{2}\hbar |\tfrac{1}{2},\tfrac{1}{2}\rangle$$

is represented by the matrix equation

$$\hbar \begin{pmatrix} 0 & 0 & 0 & \cdots \\ 0 & \frac{1}{2} & 0 & \cdots \\ 0 & 0 & -\frac{1}{2} & \cdots \\ \vdots & \vdots & \vdots & \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} = \tfrac{1}{2}\hbar \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix},$$

which is clearly correct.

When dealing with a system for which the value of j is known (e.g. the spin state of an electron: $j=\frac{1}{2}$) then it is possible to choose only the parts of the matrices corresponding to that value of j. For example, for $j=\frac{1}{2}$ we have

$$\frac{1}{\hbar}\left[\langle \tfrac{1}{2} m | \hat{J}_z | \tfrac{1}{2} m' \rangle\right] = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix},$$

& $\quad |\tfrac{1}{2},\tfrac{1}{2}\rangle \to \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\tfrac{1}{2},-\tfrac{1}{2}\rangle \to \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$

The matrix representation of the raising & lowering operators $\hat{J}_\pm$ follows from the definition of their action,

$$\hat{J}_\pm |jm\rangle = c_\pm |j\, m\pm 1\rangle$$

with $\quad c_\pm = \hbar\left[(j\mp m)(j\pm m+1)\right]^{\frac{1}{2}}.$

We have

$$\langle jm|\hat{J}_+|j'm'\rangle = c_+' \langle jm|j'\,m'+1\rangle$$

$$= c_+' \,\delta_{j,j'}\,\delta_{m,m'+1}$$

where $c_+' = c_+(j',m')$

& $\quad \langle jm|\hat{J}_-|j'm'\rangle = c_-' \langle jm|j'\,m'-1\rangle$

$$= c_-' \,\delta_{j,j'}\,\delta_{m,m'-1}$$

which describe the matrices. They are "block diagonal", i.e. have entries between the dashed lines in our figures of the matrices for $\hat{J}^2$ & $\hat{J}_z$, because they do not change the values of j.

For the case $j = \frac{1}{2}$

$$\frac{1}{\hbar}\left[\hat{J}_+\right] = \begin{pmatrix} 0 & \frac{1}{\hbar}c_+\left(j=\frac{1}{2},\, m'=-\frac{1}{2}\right) \\ 0 & 0 \end{pmatrix}$$

$\uparrow$ shorthand

$$= \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

& similarly

$$\frac{1}{\hbar}\left[\hat{J}_-\right] = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

The matrices for $\hat{J}_x$ & $\hat{J}_y$ are easily constructed from the matrices for $\hat{J}_\pm$, using

$$\boxed{\begin{aligned} \hat{J}_x &= \tfrac{1}{2}(\hat{J}_+ + \hat{J}_-) \\ \hat{J}_y &= \tfrac{1}{2i}(\hat{J}_+ - \hat{J}_-), \end{aligned}}$$

which follows from the definitions $\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y$.

Example: For $j = \frac{1}{2}$, it is easy to show (exercise):

$$[\hat{J}_x] = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad [\hat{J}_y] = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

& from before,

$$[\hat{J}_z] = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \& \quad [\hat{\underset{\sim}{J}}^2] = \frac{3}{4}\hbar^2\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

(In ass., asked to construct matrices for $j = 1$)

It is usual to introduce the Pauli matrices $\hat{\sigma}_x$, $\hat{\sigma}_y$ & $\hat{\sigma}_z$ via

$$\boxed{[\hat{\underset{\sim}{J}}] = \frac{\hbar}{2}\hat{\underset{\sim}{\sigma}}}$$

i.e.

$$\boxed{\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.}$$

(*) As mentioned above, the case $j = \frac{1}{2}$ describes the spin of the electron. Spin angular momentum represents an internal degree of freedom of a particle, which is not connected with co-ordinates. Correspondingly there is no co-ordinate representation of the state $j = \frac{1}{2}$ (or any half-integral spin state). The co-ordinate representation does however describe integral

end of L13, 30/10

values of j, corresponding to orbital AM.

3.5. Co-ordinate representation of (orbital) AM:

The components of the orbital AM operator in the co-ordinate representation follows from the definition

$$\boxed{\hat{\underset{\sim}{L}} = \hat{\underset{\sim}{x}} \times \hat{\underset{\sim}{p}}}$$

with the replacements

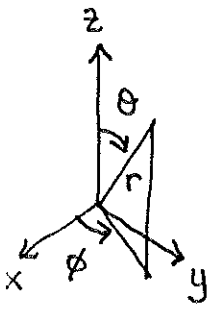
$$\boxed{\hat{\underset{\sim}{x}} \to \underset{\sim}{x} \;, \qquad \hat{\underset{\sim}{p}} \to -i\hbar\nabla}$$

In cartesian co-ordinates we have

$$\boxed{\begin{aligned} \tilde{L}_x &= -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \\ \tilde{L}_y &= -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \\ \tilde{L}_z &= -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \end{aligned}}$$

[Here I ~~have dropped~~ retained my earlier convention of writing ~'s (tildes) for an operator in the co-ordinate representation.]

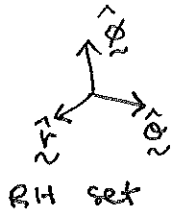
It is usual to work in spherical polar co-ordinates (r, θ, ϕ), in which case



$$\boxed{\begin{aligned} \underset{\sim}{x} &= r\hat{\underset{\sim}{r}} \qquad \leftarrow \text{unit vector, not operator!} \\ \nabla &= \hat{\underset{\sim}{r}}\frac{\partial}{\partial r} + \hat{\underset{\sim}{\theta}}\frac{1}{r}\frac{\partial}{\partial\theta} + \hat{\underset{\sim}{\phi}}\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi} \end{aligned}}$$

so

$$\tilde{\underset{\sim}{L}} = \underset{\sim}{x} \times (-i\hbar\nabla) = -i\hbar\, r\hat{\underset{\sim}{r}} \times \left[\hat{\underset{\sim}{\theta}}\frac{1}{r}\frac{\partial}{\partial\theta} + \hat{\underset{\sim}{\phi}}\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\right]$$



$$= -i\hbar\,\hat{\underset{\sim}{\phi}}\,\frac{\partial}{\partial\theta} - i\hbar\cdot(-\hat{\underset{\sim}{\theta}})\,\frac{1}{\sin\theta}\,\frac{\partial}{\partial\phi}$$

so $$\boxed{\tilde{\underset{\sim}{L}} = -i\hbar\left[\hat{\underset{\sim}{\phi}}\,\frac{\partial}{\partial\theta} - \hat{\underset{\sim}{\theta}}\,\frac{1}{\sin\theta}\,\frac{\partial}{\partial\phi}\right]}$$

depend only on angles

The Cartesian components of the operator expressed in spherical polar co-ordinates can be obtained using

$$\hat{\underset{\sim}{\theta}} = \cos\theta\cos\phi\,\hat{\underset{\sim}{x}} + \cos\theta\sin\phi\,\hat{\underset{\sim}{y}} - \sin\theta\,\hat{\underset{\sim}{z}}$$

&

$$\hat{\underset{\sim}{\phi}} = -\sin\phi\,\hat{\underset{\sim}{x}} + \cos\phi\,\hat{\underset{\sim}{y}}$$

Replacing the spherical polar unit vectors & collecting the coefficients of $\hat{\underset{\sim}{x}}$ & $\hat{\underset{\sim}{y}}$ & $\hat{\underset{\sim}{z}}$ gives

$$\boxed{\begin{aligned}\tilde{L}_x &= -i\hbar\left[-\sin\phi\,\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\,\frac{\partial}{\partial\phi}\right]\\ \tilde{L}_y &= -i\hbar\left[\cos\phi\,\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\,\frac{\partial}{\partial\phi}\right]\\ \& \quad \tilde{L}_z &= -i\hbar\,\frac{\partial}{\partial\phi}\end{aligned}}$$

depend only on angles

The representation of the operator $\hat{\underset{\sim}{L}}^2$ can be obtained using these formulae & the definition $\tilde{\underset{\sim}{L}}^2 = \tilde{L}_x^2 + \tilde{L}_y^2 + \tilde{L}_z^2$, but this approach is tedious, & so we appeal instead to the earlier result

$$\hat{\underset{\sim}{L}}^2 = \hat{\underset{\sim}{x}}^2\hat{\underset{\sim}{p}}^2 - (\hat{\underset{\sim}{x}}\cdot\hat{\underset{\sim}{p}})^2 + i\hbar\,\hat{\underset{\sim}{x}}\cdot\hat{\underset{\sim}{p}}$$

In the co-ordinate representation we have

$$\hat{\underset{\sim}{x}} \to \tilde{\underset{\sim}{x}} = \underset{\sim}{r} \quad \& \quad \hat{\underset{\sim}{p}} \to \tilde{\underset{\sim}{p}} = -i\hbar\nabla$$

(spherical polars)

& $\tilde{\underset{\sim}{x}} \cdot \tilde{\underset{\sim}{p}} = -i\hbar r \frac{\partial}{\partial r}$, so

$$\tilde{\underset{\sim}{L}}^2 = -\hbar^2 r^2 \nabla^2 + \hbar^2 r \frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \hbar^2 r \frac{\partial}{\partial r}$$

$$= -\hbar^2 r^2 \nabla^2 + \hbar^2 r^2 \frac{\partial^2}{\partial r^2} + 2\hbar^2 r \frac{\partial}{\partial r}$$

$$= -\hbar^2 r^2 \nabla^2 + \hbar^2 \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r}$$

but $$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2}\left[\frac{1}{\sin\theta} \frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta}\right) + \frac{1}{\sin^2\theta} \cdot \frac{\partial^2}{\partial \phi^2}\right]$$

so $$\boxed{\tilde{\underset{\sim}{L}}^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta}\right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2}\right]}$$

depends only on angles

Next we consider the problem of finding eigenfunctions for the momentum operators in the co-ordinate representation. The eigenvalue problem for $\tilde{\underset{\sim}{L}}^2$ consists in solving

$$\boxed{\tilde{\underset{\sim}{L}}^2 \psi_\lambda(\underset{\sim}{x}) = \hbar^2 \lambda \psi_\lambda(\underset{\sim}{x})}$$

where $\psi(\underset{\sim}{x})$ is the wavefunction of a state with orbital angular momentum squared equal to $\hbar\lambda$. Because the operator $\tilde{\underset{\sim}{L}}^2$ depends only on θ & ϕ, (& we can assume the eigenfunction depends only on θ & ϕ (& λ) & so we write $\psi_\lambda(\theta, \phi)$. We proceed by separation of variables, i.e. we look for a solution of the form

$$\boxed{\psi_\lambda(\theta, \phi) = \Theta(\theta)\Phi(\phi)}$$

(where the dependence on λ in the fns on the RHS is implicit). Substituting this form & using our expression for $\tilde{L}^2$ gives

$$-\frac{1}{\Theta}\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\frac{1}{\Phi}\frac{1}{\sin^2\theta}\frac{d^2\Phi}{d\phi^2}=\lambda$$

OR $$-\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}=\frac{\sin^2\theta}{\Theta}\left[\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\lambda\Theta\right].$$

The LHS of this equation is a function of ϕ only, & the RHS is a fn of θ only: hence both are constant, say m^2. Then

(1) $$\frac{d^2\Phi}{d\phi^2}+m^2\Phi=0$$

(2) $$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)-\frac{m^2\Theta}{\sin^2\theta}+\lambda\Theta=0.$$

The solutions to (1) are complex exponentials $e^{\pm im\phi}$. If we allow m to have positive & negative values, then we can write the solution

$$\boxed{\Phi = e^{im\phi}}.$$

The required boundary condition for a function of azimuthal angle is

$$\Phi(\phi+2\pi)=\Phi(\phi)$$

(the point $r,\theta,\phi+2\pi$ is the same as the point r,θ,ϕ). Hence we have

$$e^{2\pi m i} = 1$$

which implies

$$2\pi m = 2\pi \times \text{integer},$$

i.e. $\boxed{m \text{ is integral.}}$

end of L14, 31/10

The solution to ② is made easier by writing $\xi = \cos\theta$, $F(\xi) = \Theta[\theta(\xi)]$. Then ② becomes (exercise)

$$\boxed{\frac{d}{d\xi}\left[(1-\xi^2)\frac{dF}{d\xi}\right] - \frac{m^2 F}{1-\xi^2} + \lambda F = 0} \quad ⊛$$

Looking in a handy book on orthogonal polynomials, we note that the associated Legendre functions (m is integral) $P^m_\ell(\xi)$, for $\ell = 0, 1, \ldots$ & $0 \le |m| \le \ell$, satisfy

$$\frac{d}{d\xi}\left[(1-\xi^2)\frac{dP^m_\ell}{d\xi}\right] - \frac{m^2 P^m_\ell}{1-\xi^2} + \ell(\ell+1)P^m_\ell = 0.$$

These functions may be generated via the relation

$$P^m_\ell(\xi) = (-1)^m (1-\xi^2)^{\frac{m}{2}} \left(\frac{d}{d\xi}\right)^m P_\ell(\xi),$$

where $P_\ell(\xi)$ are the Legendre polynomials, which themselves may be generated using

$$P_\ell(\xi) = \frac{(-1)^\ell}{2^\ell \ell!}\left(\frac{d}{d\xi}\right)^\ell (1-\xi^2)^\ell.$$

Comparing ⊛ with the DE satisfied by the associated Legendre functions, we conclude that

$$F(\xi) = P^m_\ell(\xi)$$

provide eigenfunctions for our problem, with eigenvalues

$$\boxed{\lambda = \ell(\ell+1),}$$

where ℓ is integral. The possible values of m are $m = -\ell, -(\ell-1), \ldots, (\ell-1), \ell$.

In fact these are the only normalizable solutions to the eigenvalue problem for $\tilde{L}^2$, & so we have established that the eigenfunctions are the spherical harmonics

$$\psi_\lambda(\theta,\phi) = Y^m_\ell(\theta,\phi)$$

where $$\boxed{Y^m_\ell(\theta,\phi) = \left[\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}\right]^{\frac{1}{2}} P^m_\ell(\cos\theta)\cdot e^{im\phi}}$$

& where $\ell = 0, 1, 2, \ldots$ & $m = -\ell, -(\ell-1), \ldots, (\ell-1), \ell$.

The corresponding eigenvalues are

$$\hbar^2\lambda = \boxed{\hbar^2\ell(\ell+1),} \quad (\ell \text{ is integral.})$$

write it out

i.e. $\tilde{L}^2 Y^m_\ell(\theta,\phi) = \hbar^2\ell(\ell+1)Y^m_\ell(\theta,\phi)$

Note in particular that for an arbitrary AM we found the eigenvalues of $\hat{J}^2$ are $\hbar^2 j(j+1)$, where $2j$ must be integral. For orbital AM we have established that the quantum number j must be integral!

It is easy to see that $Y^m_\ell(\theta,\phi)$ are also simultaneous eigenstates for $\tilde{L}_z$. Earlier we established that $\tilde{L}_z = -i\hbar\frac{\partial}{\partial\phi}$ in the co-ordinate representation, & so

only dependence on ϕ is in $\exp(im\phi)$

$$\tilde{L}_z Y^m_\ell(\theta,\phi) = -i\hbar(im)Y^m_\ell(\theta,\phi)$$

i.e. $$\boxed{\tilde{L}_z Y^m_\ell(\theta,\phi) = \hbar m Y^m_\ell(\theta,\phi).}$$

Hence the eigenvalues are $\hbar m$, confirming what we found for an arbitrary AM.

The factors out the front in $Y^m_\ell(\theta,\phi)$ are normalization constants. The spherical harmonics are orthogonal, & with their choice of normalization they are orthonormal:

$$\int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \, Y^{*m}_\ell(\theta,\phi) \, Y^{m'}_{\ell'}(\theta,\phi) = \delta_{\ell,\ell'}\delta_{m,m'} .$$

The LHS represents an integration of $|Y^m_\ell(\theta,\phi)|^2$ over all angular variation.

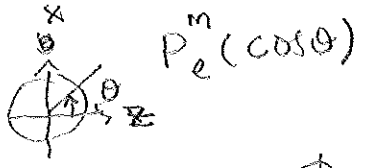
To summarise, we have established

$$\tilde{\underset{\sim}{L}}^2 Y^m_\ell(\theta,\phi) = \hbar^2 \ell(\ell+1) Y^m_\ell(\theta,\phi)$$

$$\star \quad \tilde{L}_z Y^m_\ell(\theta,\phi) = \hbar m Y^m_\ell(\theta,\phi)$$

where ℓ is integral & m is an integer st $0 \le |m| \le \ell$. This solves the eigenvalue problem for orbital AM in the co-ordinate representation.

The first few spherical harmonics may be written out:



$$Y^0_0(\theta,\phi) = (4\pi)^{-\frac{1}{2}}$$

$$Y^{\pm 1}_1(\theta,\phi) = \mp\left(\frac{3}{8\pi}\right)^{\frac{1}{2}} e^{\pm i\phi}\sin\theta$$

$$Y^0_1(\theta,\phi) = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}} \cos\theta$$

$$Y^{\pm 2}_2(\theta,\phi) = \left(\frac{15}{32\pi}\right)^{\frac{1}{2}} e^{\pm 2i\phi}\sin^2\theta$$

$$Y^{\pm 1}_2(\theta,\phi) = \mp\left(\frac{15}{8\pi}\right)^{\frac{1}{2}} e^{\pm i\phi}\cos\theta\sin\theta$$

$$Y^0_2(\theta,\phi) = \left(\frac{5}{16\pi}\right)^{\frac{1}{2}} (3\cos^2\theta - 1)$$

$$\vdots$$

3.6 The Hydrogen atom

The problem of describing the electron in a Hydrogen atom illustrates the roles of orbital angular momentum & spin in quantum theory.

For a particle moving in a central potential $V(r)$, the time-independent SE (in spherical polar co-ordinates) is

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(\underset{\sim}{x}) = E\psi(\underset{\sim}{x})$$

i.e.
$$\left\{\frac{-\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] + V(r)\right\}\psi(\underset{\sim}{x}) = E\psi(\underset{\sim}{x})$$

& comparing this with the co-ordinate-representation of the angular-momentum squared operator,

$$\underset{\sim}{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

we have

$$\boxed{\left[\frac{-\hbar^2}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\underset{\sim}{L}^2}{r^2} + 2mV(r)\right]\psi(\underset{\sim}{x}) = 2mE\psi(\underset{\sim}{x})}$$

For the Hydrogen atom we use the coulomb potential

$$\boxed{V(r) = \frac{-e^2}{4\pi\varepsilon_0 r}}$$

If we seek a separable solution,

$$\boxed{\psi(\underset{\sim}{x}) = R(r)\,\Omega(\theta,\phi),}$$

then we have

$$-\frac{1}{R}\frac{\hbar^2}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{\tilde{\underset{\sim}{L}}^2\Omega}{r^2\Omega} + 2mV = 2mE$$

OR $$-\frac{1}{R}\hbar^2\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + 2m(V-E)r^2 = -\frac{\tilde{\underset{\sim}{L}}^2\Omega}{\Omega}.$$

The LHS is a function of r only & the RHS is a fn of θ & ϕ only. Hence both must be constant, say $-\lambda$:

$$\tilde{\underset{\sim}{L}}^2\Omega = \lambda\Omega \qquad (1)$$

$$-\frac{\hbar^2}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + 2m(V-E)r^2 = -\lambda \qquad (2)$$

end of L15, 1/11

Equation (1) is our eigenvalue equation for $\tilde{\underset{\sim}{L}}^2$! Hence we immediately recognise the solutions from §3.5,

$$\boxed{\Omega = Y_\ell^m(\theta,\phi) \quad \& \quad \lambda = \hbar^2\ell(\ell+1)}$$

where ℓ is integral, & m is an integer s.t. $0 \le |m| \le \ell$.

The radial equ. (2) becomes

$$\left\{\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{2m}{\hbar^2}\left[E - V - \frac{\hbar^2}{2m}\cdot\frac{\ell(\ell+1)}{r^2}\right]\right\}R(r) = 0$$

We will not attempt to solve this equation for the Coulomb potential, but the details may be found in many QM textbooks. Here we note only the features of the solution. First, there are normalisable

solutions only for discrete values of energy E_n. The solutions, $\hat{H}$ energy eigenvalues also clearly depend on the angular momentum quantum number ℓ, & so the eigenstates can be written $R_{n\ell}$, where

$$\left\{ \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{2m}{\hbar^2}\left[E_n + \frac{e^2}{4\pi\varepsilon_0 r} - \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right]\right\} R_{n\ell} = 0$$

The solutions to this equation involve another class of orthogonal polynomials, the Laguerre polynomials. The full wavefunction for the electron in a H atom is then

$$\boxed{\psi_{n\ell m}(\underset{\sim}{x}) = R_{n\ell}(r)\, Y^m_\ell(\theta,\phi)}$$

Here we note the role played by the (orbital) AM operator & its eigenvalues in determining the wavefunction describing the Hydrogen atom. Physically, the electron in the atom has AM, which is quantized, as described by Q. #s ℓ & m. The energy ~~levels~~ of the electron is also quantized, as described by the quantum number n. It is clear from the form of the wavefunction for a stationary state, $\psi_{n\ell m}$, that the Hamiltonian operator commutes with the AM operators (this is true quite generally for QM systems).

We note finally that this theory includes only the orbital AM & not the spin AM of the electron. The Schrodinger

theory extended to include the electron spin is called the Schrodinger - Pauli theory. In this theory the dimensionality of the Hilbert space is doubled by associating two dimensions with the possible spin states of the electron. The resulting "spinor wavefunctions" representing spin up & spin down states wrt to the direction of an imposed magnetic field $\underset{\sim}{B}$ are

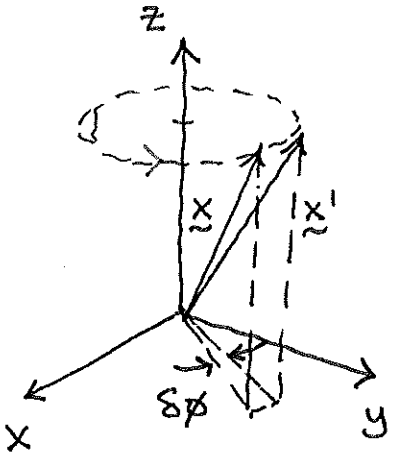
$$\psi(\underset{\sim}{x})\, e^{-i(E_{orb} + eB\hbar/2m)t/\hbar} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

& $$\psi(\underset{\sim}{x})\, e^{-i(E_{orb} - eB\hbar/2m)t/\hbar} \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

where E_{orb} is the energy in the Schrodinger theory. The interaction of the magnetic moment associated with the electron spin (this was discussed by Jim) with the external magnetic field $\underset{\sim}{B}$ changes the energy eigenvalues of the states.

3.7 AM & ROTATIONS

Consider a system with orbital AM described by an operator $\underset{\sim}{L}$, & with a wavefunction $\Psi(\underset{\sim}{x})$. We consider the effect of rotating the system through a small angle $\delta\phi$ about the z-axis, in a RH sense, i.e. CW looking along $\hat{\underset{\sim}{z}}$. If the wavefunction of the rotated system is $\Psi'(\underset{\sim}{x})$, then we must have

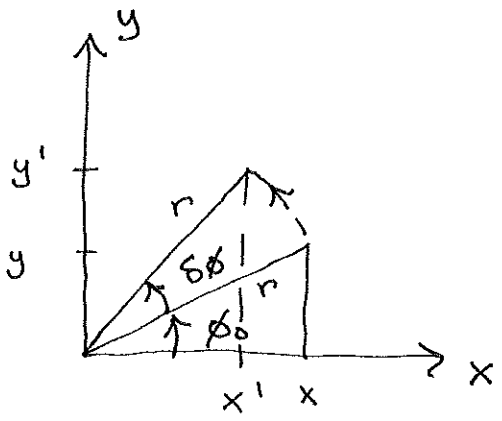


$$\boxed{\Psi'(\underset{\sim}{x}') = \Psi(\underset{\sim}{x})}$$

where $\underset{\sim}{x}'$ represents the vector $\underset{\sim}{x}$ rotated by $\delta\phi$ about z, as shown. We write

$$\boxed{\underset{\sim}{x}' = R_{\delta\phi}\,\underset{\sim}{x}}$$

to denote the rotation.



Next we determine the action of $R_{\delta\phi}$. Consider the rotation in the x-y plane, since clearly $z' = z$. We have

$$x = r\cos\phi_0, \quad y = r\sin\phi_0$$

$$\begin{aligned} x' &= r\cos(\phi_0 + \delta\phi) \\ &= r\cos\phi_0\cos\delta\phi - r\sin\phi_0\sin\delta\phi \\ &\approx x - y\,\delta\phi + O(\delta\phi^2) \end{aligned}$$

since $\cos\delta\phi \approx 1$ & $\sin\delta\phi \approx \delta\phi$ for small $\delta\phi$.

Also,

$$\begin{aligned} y' &= r\sin(\phi_0 + \delta\phi) \\ &= r\sin\phi_0\cos\delta\phi + r\cos\phi_0\sin\delta\phi \\ &\approx y + x\,\delta\phi \end{aligned}$$

Hence we have established

$$\boxed{\begin{aligned} x' &= x - y\delta\phi \\ y' &= y + x\delta\phi \\ z' &= z \end{aligned}}$$

to order $\delta\phi$. We can then identify $R\delta\phi$ with a matrix:

$$R\delta\phi = \begin{pmatrix} 1 & -\delta\phi & 0 \\ \delta\phi & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

so that $$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = R\delta\phi \begin{pmatrix} x \\ y \\ z \end{pmatrix}.$$

We expect that $R_{-\delta\phi}$ will be the inverse of $R\delta\phi$. To check this we try

$$R\delta\phi\, R_{-\delta\phi} = \begin{pmatrix} 1 & -\delta\phi & 0 \\ \delta\phi & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & \delta\phi & 0 \\ -\delta\phi & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1+\delta\phi^2 & 0 & 0 \\ 0 & 1+\delta\phi^2 & 0 \\ 0 & 0 & 1+\delta\phi^2 \end{pmatrix}$$

$$= I\,(1+\delta\phi^2) = I, \text{ to order } \delta\phi$$

Hence to order $\delta\phi$ we have

$$R_{-\delta\phi} = R\delta\phi^{-1}.$$

We want to determine an operator that produces the wavefunction of the rotated system from that of the original system, i.e.

$$\boxed{\Psi'(\underset{\sim}{x}) = \tilde{U}_z(\delta\phi)\,\Psi(\underset{\sim}{x})}$$

The labelling $\tilde{U}_z(\delta\phi)$ indicates that the operator is in the co-ordinate representation ($\sim$) & produces a rotation of an angle $\delta\phi$ about the z axis.

We already know that

$$\Psi'(\underset{\sim}{x}) = \Psi(R_{\delta\phi}^{-1}\underset{\sim}{x})$$
$$= \Psi(R_{-\delta\phi}\underset{\sim}{x})$$

so we see that

$$\tilde{U}_z(\delta\phi)\,\Psi(\underset{\sim}{x}) = \Psi(R_{-\delta\phi}\underset{\sim}{x}) \qquad \text{end of L16 3/11}$$

Q.
$$= \Psi(x+y\delta\phi, y-x\delta\phi, z)$$
$$= \Psi(x,y,z) + y\delta\phi\frac{\partial\Psi}{\partial x} - x\delta\phi\frac{\partial\Psi}{\partial y} + \mathcal{O}(\delta\phi^2)$$

Taylor expanding.

i.e. $$\tilde{U}_z(\delta\phi)\,\Psi(\underset{\sim}{x}) = \left[1 - \delta\phi\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\right]\Psi$$

to order $\delta\phi$, so we identify

Q.
$$\boxed{\tilde{U}_z(\delta\phi) = 1 - \delta\phi\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = 1 - \frac{i}{\hbar}\delta\phi\,\tilde{L}_z,}$$

recalling that $\tilde{L}_z = \{\tilde{\underset{\sim}{x}} \times \tilde{\underset{\sim}{p}}\}_z = \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \times (-i\hbar)$

More generally, for an infinitesimal rotation through an angle $\delta\phi$ about the direction defined by the unit vector $\hat{\underset{\sim}{n}}$, we have

$$\tilde{U}_{\hat{n}}(\delta\phi) = 1 - \frac{i}{\hbar}\delta\phi\,\hat{n}\cdot\tilde{L}$$

This has been established in the co-ordinate representation & involves the orbital AM operator in that representation. However, quite generally the "generator of infinitesimal rotations" for a system with arbitrary AM described by the operator $\hat{J}$ is

$$\hat{U}_{\hat{n}}(\delta\phi) = 1 - \frac{i}{\hbar}\delta\phi\,\hat{n}\cdot\hat{J}.$$

What about a rotation through a finite angle ϕ? If we write the operator for such a rotation $\hat{U}_{\hat{n}}(\phi)$, then

$$\hat{U}_{\hat{n}}(\phi+\delta\phi) = \hat{U}_{\hat{n}}(\delta\phi)\,\hat{U}_{\hat{n}}(\phi)$$

$$= \left(1 - \frac{i}{\hbar}\delta\phi\,\hat{n}\cdot\hat{J}\right)\hat{U}_{\hat{n}}(\phi)$$

relabel $\hat{U}$

$$\text{i.e.}\quad \frac{\hat{U}_{\hat{n}}(\phi+\delta\phi) - \hat{U}_{\hat{n}}(\phi)}{\delta\phi} = -\frac{i}{\hbar}\,\hat{n}\cdot\hat{J}\,\hat{U}_{\hat{n}}(\phi)$$

$$\text{i.e.}\quad \frac{1}{\hat{U}_{\hat{n}}}\frac{d\hat{U}_{\hat{n}}(\phi)}{d\phi} = -\frac{i}{\hbar}\,\hat{n}\cdot\hat{J}$$

$$\Rightarrow \quad \hat{U}_{\hat{n}} = C\,e^{-\frac{i}{\hbar}\hat{n}\cdot\hat{J}\phi}$$

But $\hat{U}_{\hat{n}}(0) = 1$, so $C = 1$, $\Rightarrow$

$$\hat{U}_{\hat{n}}(\phi) = e^{-\frac{i}{\hbar}\phi\,\hat{n}\cdot\hat{J}}$$

which is called the "generator of arbitrary rotations!"

Now consider a spin-$\frac{1}{2}$ system ($j=\frac{1}{2}$) (e.g., an electron). In this case there is a matrix representation of the spin operators & eigenstates, (but no co-ordinate representation), & in particular

$$[\hat{\underset{\sim}{J}}] = \frac{\hbar}{2}\underset{\sim}{\sigma}$$

where $\underset{\sim}{\sigma}$ are the Pauli matrices. Correspondingly there is a matrix representing the generator of arbitrary rotations,

$$\boxed{[\hat{U}_{\hat{\underset{\sim}{n}}}(\phi)] = \exp\left(-i\frac{\phi}{2}\hat{\underset{\sim}{n}}\cdot\underset{\sim}{\sigma}\right).} \quad (\text{spin } \tfrac{1}{2})$$

The RHS involves the exponential of a matrix, which is defined using the power series expansion of an exponential:

$$\exp(A) = I + A + \frac{1}{2!}A^2 + \frac{1}{3!}A^3 + \cdots$$

where I is the identity matrix. So, we have

$$[\hat{U}_{\hat{\underset{\sim}{n}}}(\phi)] = I - i\frac{\phi}{2}\hat{\underset{\sim}{n}}\cdot\underset{\sim}{\sigma} + \frac{1}{2!}(-1)\left(\frac{\phi}{2}\right)^2(\hat{\underset{\sim}{n}}\cdot\underset{\sim}{\sigma})^2 + \frac{1}{3!}(-i)^3\left(\frac{\phi}{2}\right)^3(\hat{\underset{\sim}{n}}\cdot\underset{\sim}{\sigma})^3 + \cdots$$

The Pauli matrices satisfy a vector identity for any two vectors $\underset{\sim}{A}$ & $\underset{\sim}{B}$:

$$(\underset{\sim}{\sigma}\cdot\underset{\sim}{A})(\underset{\sim}{\sigma}\cdot\underset{\sim}{B}) = \underset{\sim}{A}\cdot\underset{\sim}{B}I + i\underset{\sim}{\sigma}\cdot(\underset{\sim}{A}\times\underset{\sim}{B})$$

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[the proof is left as an exercise for a dedicated student]

Martin?

so $(\underset{\sim}{\sigma}\cdot\hat{\underset{\sim}{n}})^2 = \hat{\underset{\sim}{n}}\cdot\hat{\underset{\sim}{n}}I = 1.I = I$

Hence the series expansion for $[\hat{U}_{\underset{\sim}{\hat{n}}}(\phi)]$ becomes simpler:

$$[\hat{U}_{\underset{\sim}{\hat{n}}}] = I - i\frac{\phi}{2}\,\underset{\sim}{\hat{n}}\cdot\underset{\sim}{\sigma} - \frac{1}{2!}\left(\frac{\phi}{2}\right)^2 I - \frac{i}{3!}\left(\frac{\phi}{2}\right)^3 \underset{\sim}{n}\cdot\underset{\sim}{\sigma} + \cdots$$

$$= I\left[1 - \frac{1}{2!}\left(\frac{\phi}{2}\right)^2 - \frac{1}{4!}\left(\frac{\phi}{2}\right)^4 + \cdots\right]$$

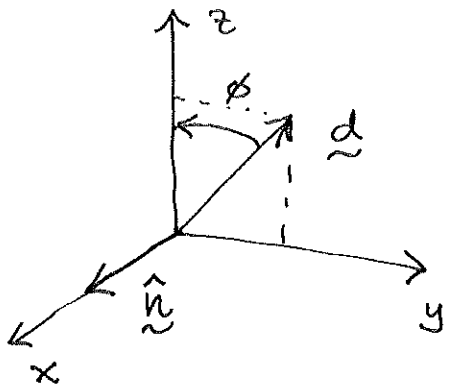
$$-i\,\underset{\sim}{\hat{n}}\cdot\underset{\sim}{\sigma}\left[\frac{\phi}{2} - \frac{1}{3!}\left(\frac{\phi}{2}\right)^3 + \cdots\right]$$

i.e. $$\boxed{[\hat{U}_{\underset{\sim}{\hat{n}}}(\phi)] = I\cos\frac{\phi}{2} - i(\underset{\sim}{\hat{n}}\cdot\underset{\sim}{\sigma})\sin\frac{\phi}{2}} \quad (\text{spin } \tfrac{1}{2})$$

To show the usefulness of this result, consider the following problem. A beam of electrons (or other $j=\frac{1}{2}$ spin particles) is prepared so that the spin is in the $+z$ direction. An experiment is performed to measure the probability of spin up / spin down along a direction at an angle ϕ to the z-axis. What is the result?

Jim used the result of this experiment repeatedly in his discussion of the principles of QM, but he did not justify the result theoretically. We are now in a position to give the justification.

First we assume the direction along which the measurement is made lies in the y-z plane. We denote the unit vector in this direction $\underset{\sim}{\hat{d}}$, as shown. The unit vector $\underset{\sim}{\hat{n}}$ associated with ϕ is then



Next consider rotating the spin-$\frac{1}{2}$ state through an angle ϕ about $\hat{n} = \hat{x}$. Then $\hat{d}$ will line up with z, & the $j = +\frac{1}{2}$ & $j = -\frac{1}{2}$ states will correspond to spin up / spin down along $\hat{d}$.

The matrix for the rotation is

$$[\hat{U}_{\hat{x}}(\phi)] = I\cos\frac{\phi}{2} - i\sigma_x \sin\frac{\phi}{2}$$

$$= \begin{pmatrix} \cos\frac{\phi}{2} & -i\sin\frac{\phi}{2} \\ -i\sin\frac{\phi}{2} & \cos\frac{\phi}{2} \end{pmatrix}$$

recalling that $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. The rotated state can be written

$$\chi' = [\hat{U}_{\hat{x}}(\phi)]\,\chi_+ \quad \leftarrow \text{spin up along } +z$$

$$= \begin{pmatrix} \cos\frac{\phi}{2} & -i\sin\frac{\phi}{2} \\ -i\sin\frac{\phi}{2} & \cos\frac{\phi}{2} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$= \begin{pmatrix} \cos\phi/2 \\ -i\sin\frac{\phi}{2} \end{pmatrix}$$

$$= \cos\frac{\phi}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix} + -i\sin\frac{\phi}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

these vectors (original system having) correspond to spin up & down along $\hat{d}$

$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hat{d}$

$\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\hat{d}$

Q

i.e. $\chi' = \cos\frac{\phi}{2}\,\chi^d_+ - i\sin\frac{\phi}{2}\,\chi^d_-$

This represents an expansion of the rotated state in terms of spin-up along $\hat{\underset{\sim}{d}}$ & spin-down along $\hat{\underset{\sim}{d}}$. Hence we identify the probability amplitudes for measuring spin-up / spin-down along $\hat{\underset{\sim}{d}}$:

$$a_+ = \cos\frac{\phi}{2} \quad \& \quad a_- = -i\sin\frac{\phi}{2}.$$

The expectation value of the measurement is

$$\langle \hat{J}_\phi \rangle = (\chi')^\dagger [\hat{J}_z](\chi')$$

$$= (\chi')^\dagger \tfrac{1}{2}\hbar\sigma_z(\chi')$$

$$= \left(\cos\tfrac{\phi}{2}, i\sin\tfrac{\phi}{2}\right)\tfrac{1}{2}\hbar\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}\cos\frac{\phi}{2}\\ -i\sin\frac{\phi}{2}\end{pmatrix}$$

$$= \tfrac{1}{2}\hbar\left(\cos^2\tfrac{\phi}{2} - \sin^2\tfrac{\phi}{2}\right) \qquad Q$$

$$= \tfrac{1}{2}\hbar\cdot|a_+|^2 + \left(-\tfrac{1}{2}\hbar\right)|a_-|^2$$

Hence the probability of spin-up along $\hat{\underset{\sim}{d}}$ is $\cos^2\frac{\phi}{2}$, & the probability of spin down along $\hat{\underset{\sim}{d}}$ is $\sin^2\frac{\phi}{2}$, as assumed by Jim.

4. IDENTICAL PARTICLES

In classical mechanics identical particles do not lose their individuality. If a number of identical particles interact, we can (in principle) "number" the particles, & follow the subsequent motion of each along its path, so that at any instant a particular particle can be identified.

In QM the situation is quite different. By virtue of the uncertainty principle, the Q path of an electron, say, does not have a precise meaning. If the position of an electron is known exactly at some time, its co-ordinates do not have exact values at a later instant. Hence we cannot "number" particles & follow precisely their paths. In QM when identical particles interact they lose their individuality: they are completely indistinguishable. This principle plays an a fundamental role in the description of QM systems consisting of identical particles.

4.1 Exchange symmetry:

Consider a system consisting of two identical particles 1 & 2. We introduce the transposition or interchange operator $\hat{P}_{12}$, which interchanges the particles (e.g. the particles may have different positions & spin states etc). The operator $\hat{P}_{12}$ ~~interchanges all of~~

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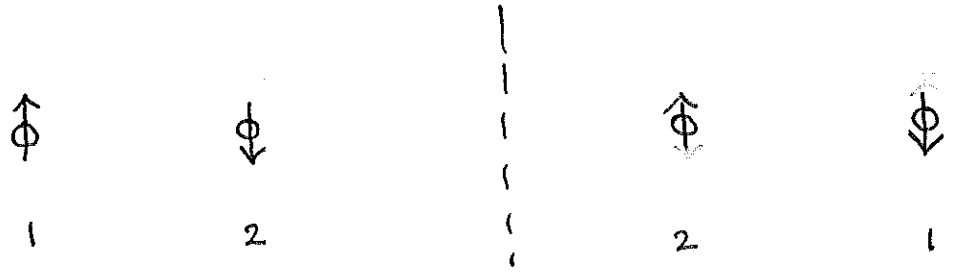
puts particle 1 at the position of 2 with the spin-state of 2, & vice versa).

e.g. electrons with spin states up and down:



What are the eigenvalues of $\hat{P}_{12}$? If $|\Psi\rangle$ denotes an eigenstate & η is the eigenvalue, then

$$\boxed{\hat{P}_{12}|\Psi\rangle = \eta|\Psi\rangle.}$$

Hence $$\hat{P}_{12}^2|\Psi\rangle = \hat{P}_{12}\hat{P}_{12}|\Psi\rangle = \eta^2|\Psi\rangle. \quad Q$$

But operating with $\hat{P}_{12}$ twice restores the system to its original state, & so

$$\hat{P}_{12}^2|\Psi\rangle = |\Psi\rangle.$$

comparing the last two equations we have

$$\boxed{\eta^2 = 1 \quad \Rightarrow \quad \eta = \pm 1}$$

Hence the eigenstates are symmetric or antisymmetric under ~~ex~~ interchange of particles ($|\Psi\rangle \to |\Psi\rangle$ or $|\Psi\rangle \to -|\Psi\rangle$). These symmetries are also referred to as even or odd symmetry under interchange, respectively.

If the system can be represented by a wavefunction, then the eigenfunction is symmetric or antisymmetric under interchange of particles.

Next note that the state obtained under interchange of particles must be physically indistinguishable from the original state (e.g. consider the two e⁻'s sketched above). Consider an energy eigenstate of the system, denoted $|E\rangle$, so that

$$\hat{H}|E\rangle = E|E\rangle$$

in our usual notation. Since the state produced by interchange of particles is physically indistinguishable, it must also be an energy eigenstate with eigenvalue E. Hence

$$\hat{H}(\hat{P}_{12}|E\rangle) = E(\hat{P}_{12}|E\rangle)$$

but also

$$\hat{P}_{12}(\hat{H}|E\rangle) = \hat{P}_{12}E|E\rangle = E(\hat{P}_{12}|E\rangle)$$

& hence $$(\hat{H}\hat{P}_{12} - \hat{P}_{12}\hat{H})|E\rangle = 0$$

$$\Rightarrow \boxed{[\hat{P}_{12}, \hat{H}] = 0 .}$$

Recall that this means $\hat{P}_{12}$ & $\hat{H}$ have simultaneous eigenstates (so the eigenstates $|I\rangle$ of $\hat{P}_{12}$ can be taken to be the $|E\rangle$).

Also, Jim Cresser established that for an observable A represented by an operator $\hat{A}$,

$$\frac{d}{dt}\langle A\rangle = \frac{i}{\hbar}\langle I|[\hat{H}, \hat{A}]|I\rangle$$

(provided $\hat{A}$ does not depend on time)

[exercise: prove this using the equ. of motion for a state vector,

$$i\hbar \frac{\partial}{\partial t}|\Psi\rangle = \hat{H}|\Psi\rangle.$$]

It follows from this equation that if an operator commutes with the Hamiltonian then its expectation values do not change with time (it is a "constant of the motion"). Applied to the interchange operator we have that if a system is initially symmetric / antisymmetric under interchange of particles, it will always be symmetric / antisymmetric under interchange. Hence the distinction between symmetric & anti-symmetric behaviour is a fundamental one, for a given system.

$$\frac{d}{dt}\langle \hat{P}_{12} \rangle = 0$$ for a given system.

Pairs of identical particles that are symmetric under interchange are called BOSONS, & those that are anti-symmetric are called FERMIONS (or Fermi particles / Bose particles):

$$\hat{P}_{12}|\Psi\rangle = |\Psi\rangle \qquad \text{BOSONS}$$

$$P_{12}|\Psi\rangle = -|\Psi\rangle \qquad \text{FERMIONS}$$

The elementary particles that are Bosons

are the photon, the mesons, & the graviton. The Fermions are the electron, the muon, the neutrinos, the nucleons, & the baryons.

Composite objects which behave (in given circumstances) as a "particle" are Fermions (Bosons) depending on whether they contain an odd number (even number) of Fermions.

The results given above concern pairs of identical particles. However, they are easily generalised to systems consisting of any number of identical particles. The state of such a system can be described by a state vector that is either invariant under interchange of any pair of particles, or changes sign under interchange of any pair of particles.

4.2 Spin-statistics theorem :

It turns out that particles that have integer spin (including $s=0$) are Bosons, whereas particles with half-integer spin are Fermions. Dirac worked out a complicated explanation based on relativistic quantum field theory, but there does not seem to be a simple explanation. This result is called the spin-statistics theorem, because Bosons & Fermions obey different statistics, as we shall see.

4.3 Many-particle wavefunctions

Because the Hamiltonian & the interchange operator commute, there exist simultaneous eigenstates of energy & the interchange operator. As shown above, these states are symmetric or antisymmetric under interchange of particles. In general, if stationary states (energy eigenstates) of a system of identical particles are found, they will not be symmetric or antisymmetric under interchange. However, it is possible to construct symmetric/antisymmetric states, as follows.

We will adopt the co-ordinate representation & talk about wavefunctions, for simplicity. Denote by $\Psi(q_1, q_2)$ an unsymmetrised eigenfunction of the Hamiltonian, where q_1 & q_2 denote spatial co-ordinates & spin states, & the position in the argument determines the state of the particle:

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$$\Psi(q_1, q_2)$$

particle 1 is in a certain state (1st position) spatial co-ordinates & spin state described by q_1.

particle 2 position in the argument

With this notation, $\Psi(q_2, q_1)$ describes the system under interchange of particles.

e.g. $\Psi(x_1, x_2) = \sin(x_1)\cos(x_2)$

position in argument determines "state"

It is easy to see that

$$\boxed{\Psi_s(q_1,q_2) = \frac{1}{\sqrt{2}}\left[\Psi(q_1,q_2) + \Psi(q_2,q_1)\right]} \quad \text{BOSONS}$$

is a symmetric wavefunction, since

$$\Psi_s(q_2,q_1) = \Psi_s(q_1,q_2).$$

The factor of $1/\sqrt{2}$ will be explained later (note that it is incorrect if $q_1 = q_2$).

The antisymmetric wavefunction is

$$\boxed{\Psi_a(q_1,q_2) = \frac{1}{\sqrt{2}}\left[\Psi(q_1,q_2) - \Psi(q_2,q_1)\right].} \quad \text{FERMIONS}$$

since $\Psi(q_2,q_1) = -\Psi(q_1,q_2)$

These wavefunctions are appropriate to describe pair of identical Bosons & Fermions respectively.

The generalisation to N identical particles is straightforward. First consider the case $N=3$. Then

$$\Psi_s = \frac{1}{\sqrt{6}}\Big[\Psi(q_1,q_2,q_3) + \Psi(q_2,q_1,q_3) + \Psi(q_2,q_3,q_1) + \Psi(q_3,q_2,q_1) + \Psi(q_3,q_1,q_2) + \Psi(q_1,q_3,q_2)\Big]$$

and

$$\Psi_a = \frac{1}{\sqrt{6}}\Big[\Psi(q_1,q_2,q_3) - \Psi(q_2,q_1,q_3) + \Psi(q_2,q_3,q_1) - \Psi(q_3,q_2,q_1) + \Psi(q_3,q_1,q_2) - \Psi(q_1,q_3,q_2)\Big].$$

The minus signs in Ψ_a appear before wavefunctions whose argument involves an

odd number of interchanges of particles. For example, $\Psi(q_2, q_1, q_3)$ is reached from $\Psi(q_1, q_2, q_3)$ by interchanging the roles of particles 1 & 2. The wavefunction $\Psi(q_2, q_3, q_1)$ can be reached from $\Psi(q_1, q_2, q_3)$ by interchanging the roles of particles 1 & 2, & then interchanging the roles of 2 & 3:

$$\Psi(q_1, q_2, q_3) \rightarrow \Psi(q_2, q_1, q_3) \rightarrow \Psi(q_2, q_3, q_1).$$

There are also other choice of ordered transpositions that would lead to the same result, but there would always be an even number of them.

This rule ensures that the wavefunction is antisymmetric under interchange of any two particles, as required. The generalisation to an arbitrary number of particles is then obvious.

Next consider a system of N identical particles, whose mutual interaction can be ignored. Let $\Psi_1, \Psi_2, \ldots$ be individual particle wavefunctions that would describe the particles if they were separate. The assumption that the mutual interaction of the particles can be ignored means that the Hamiltonian can be written as a sum of the N single particle Hamiltonians,

$$H = \sum_{\alpha=1}^{N} h_\alpha$$

where

$$\boxed{h_\alpha \Psi_\alpha(q_i) = \epsilon_\alpha \Psi_\alpha(q_i),}$$

where once again q_i denotes the co-ordinates & spin state of the particle. Then a solution to the Schrodinger equation

$$H\Psi(q_1, q_2, \cdots, q_N) = E\Psi(q_1, \cdots, q_N)$$

is

$$\Psi(q_1, q_2, \cdots, q_N) = \Psi_\alpha(q_1)\Psi_\beta(q_2)\cdots\Psi_\nu(q_N)$$

where

$$E = \epsilon_\alpha + \cdots + \epsilon_\nu.$$

The symmetric & antisymmetric wavefunctions for the $N=2$ case are

① $$\boxed{\Psi_s(q_1, q_2) = \frac{1}{\sqrt{2}}\left[\Psi_\alpha(q_1)\Psi_\beta(q_2) + \Psi_\alpha(q_2)\Psi_\beta(q_1)\right]}$$

describes Bosons

② ≠ $$\boxed{\Psi_a(q_1, q_2) = \frac{1}{\sqrt{2}}\left[\Psi_\alpha(q_1)\Psi_\beta(q_2) - \Psi_\alpha(q_2)\Psi_\beta(q_1)\right].}$$

describes fermions

For the case of N particles, the symmetric wavefunction is

$$\Psi_s(q_1, \cdots, q_N) = (N!)^{-\frac{1}{2}} \sum_P P\left[\Psi_\alpha(q_1)\Psi_\beta(q_2)\cdots\Psi_\nu(q_N)\right],$$

where $P[\cdots]$ denotes a permutation of the co-ordinates $q_1, \cdots, q_N$. There are $N!$ such permutations. The antisymmetric wavefunction is

$$\Psi_a(q_1, \cdots, q_N) = (N!)^{-\frac{1}{2}} \sum_P (-1)^p P\left[\Psi_\alpha(q_1)\cdots\Psi_\nu(q_N)\right]$$

where p is the "parity" of the permutation,

i.e. the equivalent number of transpositions. This last expression can be written in a more compact form, namely

$$\Psi_a(q_1,\dots,q_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_\alpha(q_1) & \psi_\beta(q_1) & \cdots & \psi_\nu(q_1) \\ \psi_\alpha(q_2) & & & \vdots \\ \vdots & & & \\ \psi_\alpha(q_N) & \cdots & & \psi_\nu(q_N) \end{vmatrix}$$

which is called the Slater determinant.

4.4 The Pauli exclusion principle

Going back to ② above, we see that if $\alpha = \beta$, i.e. the two particles are in the same quantum state (the same energy eigenstate, but there may be other, associated quantum numbers) then

$$\boxed{\Psi_a(q_1,q_2) = 0.}$$

This result also holds for N particles, described by the determinant above. If among the sets of numbers $\alpha, \beta, \dots, \nu$ two or more are the same, then two or more columns in the matrix are identical & the determinant of the matrix is zero.

* NB also the normalisation of the symm. wavefn is wrong if two or more of the α's are same

Since the antisymmetric wavefunction describes fermions, the conclusion is that for a system of identical fermions, no two (or more) particles can be in the

same state at the same time. This is the Pauli exclusion principle, first formulated by W. Pauli in 1925. The exclusion principle accounts for the electronic structure of atoms, & hence the stability of matter, the nature of chemical bonds ... in the words of R. Feynman, "almost all the peculiarities of the material world." (end of L20, 10/11)

4.5 Spin states for two spin-$\frac{1}{2}$ particles

Consider a system consisting of two electrons. Each can be in the spin up or spin down configuration, with respect to some given axis. We will label the up state as α & the down state β & number the electrons 1 & 2, so that

$$\alpha(1)\,\beta(2)$$

denotes the situation that electron 1 has spin up & electron 2 has spin down. The possible combinations of spin states are then

$$\alpha(1)\alpha(2),\quad \alpha(1)\beta(2),\quad \beta(1)\alpha(2),\quad \beta(1)\beta(2).$$

There are four possible ways to combine these states so that the result has a definite exchange symmetry. They are:

SYMMETRIC

$\alpha(1)\,\alpha(2)$

$\frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2) + \alpha(2)\beta(1)\right]$

$\beta(1)\,\beta(2)$

ANTISYMMETRIC

$\frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2) - \alpha(2)\beta(1)\right]$

The three symmetric states are called triplet states, & the single antisymmetric state is called a singlet state.

The total wavefunction for the two electrons is the product of a spatial function ψ & one of the possible spin states χ. The total wavefunction must be antisymmetric under interchange of positions & spin states. Hence if the electrons are in the singlet spin state, the spatial part of the wavefunction must be symmetric. If the electrons are in one of the triplet states, the spatial function ψ must be antisymmetric.

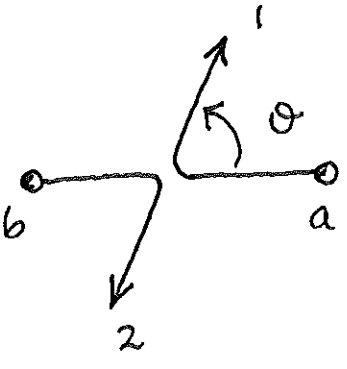
4.6 Elastic scattering of identical particles

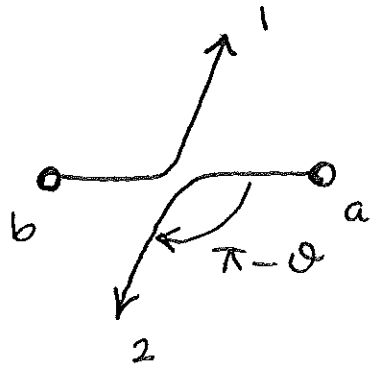
Elastic scattering experiments illustrate the quantum mechanics of identical particles. Consider an elastic collision between two identical particles in the COM frame of the particles, so that before & after collision the particles are moving in opposite directions with the same speed. We will begin by restricting ourselves to a discussion of the collision of spinless ($j=0$) Bosons, because of the complications introduced by needing to consider all possible spin states in more general collisions.

Consider two situations –

Ⓐ: particle a is deflected by θ (& b is deflected by $\pi-\theta$)

Ⓑ: particle a is deflected by $\pi-\theta$ (& b is deflected by θ)





Classically these situations are distinct events (e.g. colour one particle red & the

other blue, & see which ends up where).

Hence the probability for detecting a particle at 1 (& one at 2) is

$$\boxed{P_{class}(\theta) = p(\theta) + p(\pi-\theta),}$$

where $p(\theta)$ is the probability for scattering through an angle θ.

Quantum mechanically we cannot distinguish Ⓐ & Ⓑ: hence they are not distinct events & we do not add the individual probabilities for their occurrence. Instead, the scattering probability is the modulus squared of a probability amplitude which is a sum of probability amplitudes for the possibilities Ⓐ & Ⓑ:

$$P_{QM} = |f_Ⓐ(\theta) + f_Ⓑ(\theta)|^2.$$

If you replace θ by $\pi-\theta$ in case Ⓐ then Ⓑ is obtained. This tells us that

$$|f_Ⓐ(\pi-\theta)|^2 = |f_Ⓑ(\theta)|^2.$$

But we also know that replacing θ by $\pi-\theta$ amounts to interchanging the roles of the particles. Since they are Bosons we conclude

$$f_Ⓐ(\pi-\theta) = + f_Ⓑ(\theta).$$

Hence we have the QM result for the collision of identical spinless Bosons:

identical spinless bosons

$$\boxed{P_{QM}(\theta) = |f(\theta) + f(\pi-\theta)|^2}$$

(where we have dropped the Ⓐ). This can be compared with the classical result, which re-expressed in terms of probability amplitudes is

$$\boxed{P_{class}(\theta) = |f(\theta)|^2 + |f(\pi-\theta)|^2.}$$

If we put $\theta = \frac{\pi}{2}$ in the formulae, we get

$$\boxed{P_{class}\left(\tfrac{\pi}{2}\right) = 2\,|f(\tfrac{\pi}{2})|^2} \quad \& \quad \boxed{P_{QM}\left(\tfrac{\pi}{2}\right) = 4\,|f(\tfrac{\pi}{2})|^2,}$$

so the QM result for spinless Bosons is twice the classical result. Experiments confirm that the QM result is correct.

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Next consider the scattering problem for identical spin $\frac{1}{2}$ particles. We have seen that the spin part of the wavefunction describing two electrons can be in a singlet spin state, or in a triplet spin state. If the system is in the singlet spin state, the spin part of the wavefn is antisymmetric, & so the spatial part of the wavefunction must be symmetric, for the overall wavefunction to be anti-symmetric (as required for two fermions). Hence the scattering amplitude takes the form

$$f_s(\theta) + f_s(\pi-\theta).$$

On the other hand if the two electrons

are in a triplet state then the spatial part of the wavefunction must be anti-symmetric, & so the scattering amplitude takes the form

$$f_t(\theta) - f_t(\pi-\theta).$$

For "unpolarised" colliding particles (i.e. randomly oriented spins) the probability of being in the triplet state is three times that of being in the singlet state, & so we obtain the probability of scattering thru θ

$$\boxed{P(\theta) = \frac{1}{4}\left|f_s(\theta) + f_s(\pi-\theta)\right|^2 + \frac{3}{4}\left|f_t(\theta) - f_t(\pi-\theta)\right|^2.}$$

for spin-independent central interactions we have

$$f_s(\theta) = f_t(\theta) = f(\theta),$$

& then for $\theta = \frac{\pi}{2}$ we have

$$\boxed{P\left(\tfrac{\pi}{2}\right) = \left|f\left(\tfrac{\pi}{2}\right)\right|^2,}$$

which is half the classical result, & which is confirmed by experiment. Hence elastic scattering of identical particles illustrates the interchange symmetries of Bosons & Fermions, & the distinction with classical behaviour.

4.7 Operator approach to systems of identical particles

Many-particle states for weakly-interacting particles can be written

$$|n_1, n_2, \ldots, n_k, \ldots\rangle ,$$

where n_k is the number of particles in the k^{th} one-particle state. We assume that the set of all possible such states is an orthonormal set:

$$\langle n_1', n_2', \ldots, n_k', \ldots | n_1, n_2, \ldots, n_k, \ldots\rangle = \delta_{n_1' n_1}\, \delta_{n_2' n_2} \cdots \delta_{n_k' n_k} \cdots$$

Bosons:

For systems of Bosons we define creation & annihilation operators

$$\hat{a}_k |n_1, n_2, \ldots, n_k, \ldots\rangle = n_k^{\frac{1}{2}} |n_1, n_2, \ldots, n_k - 1, \ldots\rangle$$

$$\hat{a}_k^\dagger |n_1, n_2, \ldots, n_k, \ldots\rangle = (n_k + 1)^{\frac{1}{2}} |n_1, n_2, \ldots, n_k + 1, \ldots\rangle$$

which change the number of particles in one of the one-particle states. (cf. the creation & annihilation operators for the SHO). We also require

$$\hat{a}_k |n_1, n_2, \ldots, 0, \ldots\rangle = 0 ,$$

(0 in the k^{th} place)

since you can't destroy a particle that isn't there.

These operators satisfy the commutation relation

$$\boxed{[\hat{a}_k, \hat{a}_\ell^\dagger] = \delta_{k\ell}}$$

To see this, consider two cases.

If $k \neq \ell$,

$$\hat{a}_k \hat{a}_\ell^\dagger |n_1, n_2, \ldots, n_k, \ldots, n_\ell, \ldots\rangle$$

$$= \hat{a}_k (n_\ell + 1)^{\frac{1}{2}} |n_1, n_2, \ldots, n_k, \ldots, n_\ell + 1, \ldots\rangle$$

$$= n_k^{\frac{1}{2}} (n_\ell + 1)^{\frac{1}{2}} |n_1, n_2, \ldots, n_k - 1, \ldots, n_\ell + 1, \ldots\rangle$$

&

$$\hat{a}_\ell^\dagger \hat{a}_k |n_1, n_2, \ldots, n_k, \ldots, n_\ell, \ldots\rangle$$

$$= \hat{a}_\ell^\dagger n_k^{\frac{1}{2}} |n_1, n_2, \ldots, n_k - 1, \ldots, n_\ell, \ldots\rangle$$

$$= (n_\ell + 1)^{\frac{1}{2}} n_k^{\frac{1}{2}} |n_1, n_2, \ldots, n_k - 1, \ldots, n_\ell + 1, \ldots\rangle$$

so we have

$$\hat{a}_k \hat{a}_\ell^\dagger |n_1, n_2, \ldots, n_k, \ldots, n_\ell, \ldots\rangle$$

$$= \hat{a}_\ell^\dagger \hat{a}_k |n_1, n_2, \ldots, n_k, \ldots, n_\ell, \ldots\rangle$$

i.e. $\hat{a}_k \hat{a}_\ell^\dagger = \hat{a}_\ell^\dagger \hat{a}_k$, in operator terms

or $[\hat{a}_k, \hat{a}_\ell^\dagger] = 0$, for $k \neq \ell$

If $k = \ell$,

$$\hat{a}_k \hat{a}_k^\dagger |n_1, n_2, \ldots, n_k, \ldots\rangle$$

$$= \hat{a}_k (n_k + 1)^{\frac{1}{2}} |n_1, n_2, \ldots, n_k + 1, \ldots\rangle$$

$$= (n_k + 1)^{\frac{1}{2}} (n_k + 1)^{\frac{1}{2}} |n_1, n_2, \ldots, n_k + 1, \ldots\rangle$$

$$= (n_k + 1) |n_1, n_2, \ldots, n_k + 1, \ldots\rangle$$

$$\hat{a}_k^\dagger \hat{a}_k \,|n_1, n_2, \ldots, n_k, \ldots\rangle$$

$$= \hat{a}_k^\dagger \, n_k^{\frac{1}{2}} \,|n_1, n_2, \ldots, n_k - 1, \ldots\rangle$$

$$= n_k^{\frac{1}{2}} \, n_k^{\frac{1}{2}} \,|n_1, n_2, \ldots, n_k, \ldots\rangle = n_k \,|n_1, n_2, \ldots, n_k, \ldots\rangle \quad (*)$$

so $$\left(\hat{a}_k \hat{a}_k^\dagger - \hat{a}_k^\dagger \hat{a}_k\right) |n_1, n_2, \ldots, n_k, \ldots\rangle$$

$$= \left[(n_k + 1) - n_k\right] |n_1, n_2, \ldots, n_k, \ldots\rangle$$

$$= 1 \cdot |n_1, n_2, \ldots, n_k, \ldots\rangle$$

or $$\left[\hat{a}_k, \hat{a}_k^\dagger\right] = 1$$

Hence we have established $\left[\hat{a}_k, \hat{a}_\ell^\dagger\right] = \delta_{k\ell}$.

The equation $(*)$, i.e.

$$\boxed{\hat{a}_k^\dagger \hat{a}_k \,|n_1, n_2, \ldots, n_k, \ldots\rangle = n_k \,|n_1, n_2, \ldots, n_k, \ldots\rangle}$$

established that $\hat{a}_k^\dagger \hat{a}_k$ is the "number operator", i.e.

$$\boxed{\hat{N}_k = \hat{a}_k^\dagger \hat{a}_k}$$

returns the number of particles in the k^{th} one-particle state.

It is possible to construct a Hamiltonian using the number operator:

$$\hat{H} = \sum_k \hat{N}_k E_k = \sum_k \hat{a}_k^\dagger \hat{a}_k E_k,$$

where E_k is the energy of the k^{th} one-particle state.

end of L22, 14/11

Finally, we can construct an arbitrary state

from the "vacuum" state

$$|\text{vac}\rangle = |0_1, 0_2, \ldots, 0_k, \ldots\rangle$$

by repeat operation with the creation operator:

$$|n_1, n_2, \ldots, n_k, \ldots\rangle = \frac{(\hat{a}_1^\dagger)^{n_1}}{(n_1!)^{\frac{1}{2}}} \frac{(\hat{a}_2^\dagger)^{n_2}}{(n_2!)^{\frac{1}{2}}} \cdots \frac{(\hat{a}_k^\dagger)^{n_k}}{(n_k!)^{\frac{1}{2}}} \cdots \cdot |\text{vac}\rangle$$

Fermions:

For Fermions we introduce the anti-commutator bracket $[\ ]_+$:

$$[\hat{A}, \hat{B}]_+ = \hat{A}\hat{B} + \hat{B}\hat{A}$$

& the creation & annihilation operators $\hat{c}_k^\dagger, \hat{c}_k$ satisfy

$$[\hat{c}_k, \hat{c}_\ell]_+ = \hat{c}_k \hat{c}_\ell + \hat{c}_\ell \hat{c}_k = 0 \quad (1)$$

$$[\hat{c}_k^\dagger, \hat{c}_\ell^\dagger]_+ = \hat{c}_k^\dagger \hat{c}_\ell^\dagger + \hat{c}_\ell^\dagger \hat{c}_k^\dagger = 0 \quad (2)$$

$$[\hat{c}_k, \hat{c}_\ell^\dagger]_+ = \hat{c}_k \hat{c}_\ell^\dagger + \hat{c}_\ell^\dagger \hat{c}_k = \delta_{k\ell} \quad (3)$$

Rather than justify these relations a priori, we will see that they represent the correct behaviour for Fermions.

First note that setting $k = \ell$ in (1) & (2) gives

$$\hat{c}_k \hat{c}_k = 0 \quad (4)$$

& $$\hat{c}_k^\dagger \hat{c}_k^\dagger = 0 \quad (5)$$

The second of these relations says that you

can't put two Fermions in the same one-particle state, consistent with the exclusion principle. The first also says you can only have (at most) one particle in each state.

Alternatively, introduce the number operator

$$\boxed{\hat{N}_k = \hat{c}_k^\dagger \hat{c}_k}$$

& note that

$$\begin{aligned}
\hat{N}_k^2 &= \hat{c}_k^\dagger \hat{c}_k \hat{c}_k^\dagger \hat{c}_k \\
&= \hat{c}_k^\dagger (1 - \hat{c}_k^\dagger \hat{c}_k) \hat{c}_k \qquad \text{using } (2) \\
&= \hat{c}_k^\dagger \hat{c}_k - \hat{c}_k^\dagger \hat{c}_k^\dagger \hat{c}_k \hat{c}_k \\
&= \hat{c}_k^\dagger \hat{c}_k \qquad \text{using } (4), (5) \\
&= \hat{N}_k
\end{aligned}$$

i.e. $\boxed{\hat{N}_k^2 = \hat{N}_k}$

operating on an arbitrary state $|n_1, n_2, \ldots, n_k, \ldots\rangle$ implies

$$n_k^2 = n_k \Rightarrow n_k(n_k - 1) = 0$$

i.e. $\boxed{n_k = 0, 1}$ for every k

i.e. each one-particle state can only have zero or one particles, consistent with the exclusion principle.

For a single one-particle state we can write down an explicit matrix representation of the operators & states. The states can be

written

$$|0\rangle \to \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle \to \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Explicit matrices for $\hat{c}$, $\hat{c}^\dagger$ & $\hat{N}$ are

$$\hat{c} \to \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \hat{c}^\dagger \to \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$N = \hat{c}^\dagger \hat{c} \to \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

The following equations are then seen to be satisfied by the matrix / vector representatives:

$$\hat{c}\,|n\rangle = n\,|1-n\rangle, \quad \hat{c}^\dagger\,|n\rangle = (1-n)\,|1-n\rangle.$$

The explicit action of the creation & annihilation operators is more complicated (for the general multi-state system) than for Bosons. To understand why this is so, recall that for Bosons

$$\hat{a}_k^\dagger \hat{a}_{k+1}^\dagger\,|n_1, n_2, \ldots, n_k, n_{k+1}, \ldots\rangle$$

$$= \hat{a}_{k+1}^\dagger \hat{a}_k^\dagger\,|n_1, n_2, \ldots, n_k, n_{k+1}, \ldots\rangle.$$

The order of operation on different one-particle states is unimportant: the states are independent. This is no longer true for Fermions: the anticommutation relation ② implies

$$\hat{c}_k^\dagger \hat{c}_{k+1}^\dagger\,|n_1, n_2, \ldots, n_k, n_{k+1}, \ldots\rangle$$

$$= -\,\hat{c}_{k+1}^\dagger \hat{c}_k^\dagger\,|n_1, n_2, \ldots, n_k, n_{k+1}, \ldots\rangle.$$

Hence the actions of the operators on different one particle states is no longer independent.

The correct statement of the actions is

$$\hat{c}_k |n_1, n_2, \ldots, n_k, \ldots\rangle = \theta_k n_k |n_1, n_2, \ldots, 1-n_k, \ldots\rangle$$

$$\& \quad \hat{c}_k^\dagger |n_1, n_2, \ldots, n_k, \ldots\rangle = \theta_k (1-n_k) |n_1, n_2, \ldots, 1-n_k, \ldots\rangle$$

where $\theta_k = (-1)^{\nu_k}$

with $\nu_k = \sum_{j=1}^{k-1} n_j$.

This shows how the action of the operators depends on the number of particles in the other states. As with Bosons, an arbitrary state can be constructed by repeat operation with $\hat{c}_k^\dagger$'s.

APPENDICES

1. Proof of vector ID for Pauli matrices
2. Proof of non-commutation $\Rightarrow$ uncertainty relation

APPENDIX:

RTP $(\underset{\sim}{\sigma}\cdot\underset{\sim}{A})(\underset{\sim}{\sigma}\cdot\underset{\sim}{B}) = \underset{\sim}{A}\cdot\underset{\sim}{B} + i\underset{\sim}{\sigma}\cdot(\underset{\sim}{A}\times\underset{\sim}{B})$

For Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

It is easy to verify these matrices satisfy:

$$\sigma_i\sigma_k + \sigma_k\sigma_i = 2\delta_{ik} \qquad (1)$$

&

$$\sigma_i\sigma_j = i\varepsilon_{ijk}\sigma_k + \delta_{ij}\sigma_i\sigma_j \qquad (2)$$

(These are obvious)

Hence

$$(\underset{\sim}{\sigma}\cdot\underset{\sim}{A})(\underset{\sim}{\sigma}\cdot\underset{\sim}{B}) = \sigma_i\sigma_j A_i B_j$$

$$= (2\delta_{ij} - \sigma_j\sigma_i) A_i B_j \quad \text{by (1)}$$

$$= 2A_iB_i - \sigma_j\sigma_i A_i B_j$$

$$= 2A_iB_i - i\varepsilon_{jik}\sigma_k A_i B_j$$

$$- \delta_{ij}\sigma_j\sigma_i A_i B_j \quad \text{by (2)}$$

Recall

$$\varepsilon_{ijk} = \begin{cases} 0 & \text{repeat index} \\ 1 & \text{even perm of } (1,2,3) \\ -1 & \text{odd perm of } (1,2,3) \end{cases}$$

$$= 2A_iB_i - \sigma_i^2 A_iB_i$$

$$+ i\varepsilon_{kij}\sigma_k A_i B_j$$

$$= A_iB_i + i\underset{\sim}{\sigma}\cdot(\underset{\sim}{A}\times\underset{\sim}{B}) \quad \text{since } \sigma_i^2 = 1 \text{ by (1)}$$

$$= \underset{\sim}{A}\cdot\underset{\sim}{B} + i\underset{\sim}{\sigma}\cdot(\underset{\sim}{A}\times\underset{\sim}{B}) \quad \blacksquare$$

$[\hat{A},\hat{B}] = iB$

$\bar{A} = \hat{A} - \langle A \rangle$ and $(\Delta A)^2 = \langle \bar{A}^2 \rangle$

$\bar{B} = \hat{B} - \langle B \rangle$ $\quad (\Delta B)^2 = \langle \bar{B}^2 \rangle$

$$[\bar{A},\bar{B}] = [\hat{A} - \langle A \rangle, \hat{B} - \langle B \rangle]$$

$$= [\hat{A},\hat{B}]$$

consider $\hat{C} = \bar{A} + i\lambda\bar{B}$

where λ is real

$$\hat{C}^\dagger = \bar{A} - i\lambda\bar{B}$$

$$\langle \hat{C}\hat{C}^\dagger \rangle = \langle \Psi | \hat{C}\hat{C}^\dagger | \Psi \rangle \geq 0$$

since it is the inner product of $\hat{C}^\dagger|\Psi\rangle$ with the corresponding bra $\langle \hat{C}\hat{C}^\dagger \rangle$

$$\langle (\bar{A} + i\lambda\bar{B})(\bar{A} - i\lambda\bar{B}) \rangle$$

$$= \langle \bar{A}^2 + \lambda^2\bar{B}^2 - i\lambda[\bar{A},\bar{B}] \rangle \geq 0$$

$$\Rightarrow \langle \bar{A}^2 \rangle + \lambda^2 \langle \bar{B}^2 \rangle - i\lambda \langle [\bar{A},\bar{B}] \rangle \geq 0$$

i.e. $(\Delta A)^2 + \lambda^2(\Delta B)^2 - i\lambda\langle[\bar{A},\bar{B}]\rangle \geq 0$

Let $f(\lambda) = (\Delta A)^2 + \lambda^2(\Delta B)^2 - i\lambda\langle[\bar{A},\bar{B}]\rangle$

$$f'(\lambda) = -i\langle[\bar{A},\bar{B}]\rangle + 2\lambda(\Delta B)^2$$

so $f'(\lambda) = 0$ for $\lambda = \lambda_0 = \dfrac{i\langle[\bar{A},\bar{B}]\rangle}{2(\Delta B)^2}$

so $f(\lambda_0) = (\Delta A)^2 + - \Delta B^2 \cdot \frac{\langle [\bar{A}, \bar{B}] \rangle^2}{4(\Delta B)^4}$

$$- i \langle [\bar{A}, \bar{B}] \rangle \cdot i \frac{\langle [\bar{A}, \bar{B}] \rangle}{2(\Delta B)^2}$$

$$= (\Delta A)^2 + \frac{1}{4} \frac{\langle [\bar{A}, \bar{B}] \rangle^2}{(\Delta B)^2}$$

But $f(\lambda_0) \geq 0$, so

$$(\Delta A)^2 (\Delta B)^2 \geq -\frac{1}{4} \left(\langle [\bar{A}, \bar{B}] \rangle \right)^2$$

but $[\hat{A}, \hat{B}] = i\hat{D}$

$$(\Delta A)^2 (\Delta B)^2 \geq \frac{1}{4} \left(\langle \hat{D} \rangle \right)^2$$

or $(\Delta A)(\Delta B) \geq \frac{1}{2} |\langle \hat{D} \rangle|$

e.g. $[\hat{x}, \hat{p}_x] = i\hbar$

so $\Delta x \, \Delta p_x \geq \frac{1}{2}\hbar$

PHYS304 QUANTUM PHYSICS II 2000

Assignment 5 due Friday October 20

This assignment introduces the "momentum representation," and shows its relationship to the co-ordinate representation.

Consider a particle undergoing one-dimensional motion in the x direction. The momentum eigenstates of the particle must satisfy

$$\hat{p}|p\rangle = p|p\rangle. \tag{1}$$

(a) Write down the co-ordinate representation version of this equation and solve it to show that the wavefunction corresponding to a momentum eigenstate of a particle is

$$\psi_p(x) = \langle x|p\rangle = C\exp(ipx/\hbar), \tag{2}$$

where C is a normalisation constant. [This wavefunction is not strictly normalisable, because the restriction to a specific momentum means that the wavefunction spreads out over all x. However, the normalisation $C = (2\pi\hbar)^{-1/2}$ can be justified on certain grounds. You do not have to derive this value of C, but you can assume it for **(b)** and **(c)** below.]

The momentum representation is concerned with the "wavefunction in momentum space,"

$$\phi(p) = \langle p|\psi\rangle, \tag{3}$$

where $|\psi\rangle$ is an arbitrary state of the particle. By construction, $|\phi(p)|^2 dp$ is the probability that the particle has momentum in the range $(p, p+dp)$.

(b) Expand the right-hand side of (3) in position basis states and use the result of part **(a)** to establish

$$\phi(p) = (2\pi\hbar)^{-1/2}\int_{-\infty}^{\infty} dx\, e^{-ipx/\hbar}\psi(x). \tag{4}$$

You may recognise this equation means that $\phi(p)$ and $\psi(x)$ are related by a Fourier transform.

(c) Following a similar procedure to **(b)**, show that

$$\psi(x) = (2\pi\hbar)^{-1/2}\int_{-\infty}^{\infty} dp\, e^{ipx/\hbar}\phi(p). \tag{5}$$

PHYS304 QUANTUM PHYSICS II 2000

Assignment 6 due Friday October 27

1. Use the results of lectures to show that the matrix elements corresponding to the momentum operator for the simple harmonic oscillator are given by

$$[\langle n|\hat{p}|m\rangle] = i\left(\frac{m\hbar\omega}{2}\right)^{\frac{1}{2}} \begin{pmatrix} 0 & -\sqrt{1} & 0 & 0 & \dots \\ \sqrt{1} & 0 & -\sqrt{2} & 0 & \dots \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ \cdot & \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \cdot & \end{pmatrix}.$$

2. Consider the matrix elements corresponding to the square of the position operator, $\langle n|\hat{x}^2|m\rangle$, for the SHO. Expanding in energy eigenstates $|l\rangle$ we have

$$\langle n|\hat{x}^2|m\rangle = \sum_{l=0}^{\infty}\langle n|\hat{x}|l\rangle\langle l|\hat{x}|m\rangle. \tag{1}$$

   This equation can be interpreted as meaning that the matrix corresponding to $\hat{x}^2$ is the matrix corresponding to $\hat{x}$ times itself. With this knowledge and using the result for the matrix representation of the position operator given in lectures, determine the matrix corresponding to $\hat{x}^2$.

3. In lectures it was shown that the creation and annihilation operators $\hat{a}^\dagger$ and $\hat{a}$ for the simple harmonic oscillator satisfy

$$\hat{a}\hat{a}^\dagger = \frac{\widehat{H}}{\hbar\omega} + \frac{1}{2} \quad \text{and} \quad \hat{a}^\dagger\hat{a} = \frac{\widehat{H}}{\hbar\omega} - \frac{1}{2}. \tag{2}$$

   Use (2) to establish the commutation relations

$$[\hat{a}, \hat{a}^\dagger] = 1, \quad [\hat{a}, \widehat{H}] = \hbar\omega\hat{a}, \quad [\hat{a}^\dagger, \widehat{H}] = -\hbar\omega\hat{a}^\dagger.$$

In the momentum representation the expectation value of an operator $\widehat{\Omega}$ is

$$\langle \Omega \rangle = \int_{-\infty}^{\infty} dp\, \phi^*(p) \widetilde{\Omega} \phi(p), \tag{6}$$

where $\widetilde{\Omega}$ is the momentum representation of the operator. Because the expectation value is the average, we must have

$$\langle p \rangle = \int_{-\infty}^{\infty} dp\, p |\phi(p)|^2, \tag{7}$$

and comparing this with (6) we infer that $\widetilde{p} = p$, i.e. in the momentum representation the action of the momentum operator is multiplication by momentum.

The wavefunction in momentum space for a particle with a known position is

$$\phi_x(p) = \langle p|x \rangle, \tag{8}$$

and taking the complex conjugate of (2) we have

$$\phi_x(p) = (2\pi\hbar)^{-1/2} \exp(-ipx/\hbar). \tag{9}$$

Because $\phi_x(p)$ is the eigenfunction for the position operator in the momentum representation, $\widetilde{x}$, we must have

$$\widetilde{x}\phi_x(p) = x\phi_x(p). \tag{10}$$

(d) Use (9) together with (10) to guess the form for the position operator in the momentum representation.

(e) Show that the fundamental commutation relation

$$[\widetilde{x}, \widetilde{p}] = i\hbar \tag{11}$$

is satisfied for the position and momentum operators in the momentum representation.

PHYS304 QUANTUM PHYSICS II 2000

Assignment 7 due Friday November 10

1. A system is prepared in the state $|jm\rangle$.

   (a) Calculate the expectation values $\langle \hat{J}_z \rangle$, $\langle \hat{J}_x \rangle$ and $\langle \hat{J}_x^2 \rangle$. [Hint: you may find it useful to use $\hat{J}_x = \frac{1}{2}(\hat{J}_+ + \hat{J}_-)$.]

   (b) What are the possible outcomes of measurements of the z component of momentum, the x component of momentum, and the square of the x component of momentum of the system?

   (c) Give a brief physical explanation of the results for $\langle \hat{J}_x \rangle$ and $\langle \hat{J}_x^2 \rangle$ from part (a) (e.g. if one of the expectation values is zero and the other is not, why?).

2. (a) Construct the matrix representation of the angular momentum operator for $j = 1$. Specifically, assume the forms for the eigenstates

$$|1\,1\rangle \rightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |1\,0\rangle \rightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |1\,{-1}\rangle \rightarrow \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

   and use

$$\begin{aligned} \hat{J}_z|jm\rangle &= \hbar m|jm\rangle, \\ \hat{J}_+|jm\rangle &= \hbar[(j-m)(j+m+1)]^{1/2}|j\,m+1\rangle, \\ \hat{J}_-|jm\rangle &= \hbar[(j+m)(j-m+1)]^{1/2}|j\,m-1\rangle \end{aligned}$$

   to construct the 3×3 matrices representing $\hat{J}_x$, $\hat{J}_y$ and $\hat{J}_z$.

   (b) Confirm the matrices satisfy the commutation relation

$$[\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z.$$

PHYS304 QUANTUM PHYSICS II 2000

Assignment 8 due Friday November 17

1. Assume that $\hat{\mathbf{J}}_1$ and $\hat{\mathbf{J}}_2$ are two independent angular momenta. The assumption of independence implies

$$[\hat{\mathbf{J}}_1, \hat{\mathbf{J}}_2] = 0.$$

Show that $\hat{\mathbf{J}} = \hat{\mathbf{J}}_1 + \hat{\mathbf{J}}_2$ is also an angular momentum, i.e. its components satisfy the commutation relations

$$[\hat{J}_x, \hat{J}_y] = i\hbar J_z, \quad [\hat{J}_y, \hat{J}_z] = i\hbar J_x, \quad [\hat{J}_z, \hat{J}_x] = i\hbar J_y.$$

(6)

2. Using the properties of the Pauli matrices

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I$$

and

$$\sigma_x\sigma_y = i\sigma_z, \quad \sigma_y\sigma_z = i\sigma_x, \quad \sigma_z\sigma_x = i\sigma_y,$$

show that the Pauli matrices satisfy the vector identity

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$$(\boldsymbol{\sigma} \cdot \mathbf{A})(\boldsymbol{\sigma} \cdot \mathbf{B}) = \mathbf{A} \cdot \mathbf{B} I + i\boldsymbol{\sigma} \cdot (\mathbf{A} \times \mathbf{B}).$$

3. Recall the problem addressed in lectures, of determining the expectation value for the spin measured along a direction $\hat{\mathbf{d}} = (0, \sin\phi, \cos\phi)$ for a spin $\frac{1}{2}$ particle *prepared with its spin in the z direction.* The projection of the spin operator in the $\hat{\mathbf{d}}$ direction is

$$\begin{aligned} \hat{\mathbf{J}} \cdot \hat{\mathbf{d}} &= \hat{J}_z \cos\phi + \hat{J}_y \sin\phi \\ &= \hat{J}_z \cos\phi + \frac{1}{2i}(\hat{J}_+ - \hat{J}_-) \sin\phi. \end{aligned}$$

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Use this form to evaluate the expectation value of $\hat{\mathbf{J}} \cdot \hat{\mathbf{d}}$, confirming the result found in lectures.

(a). The co-ordinate representation version of the equation is

$$-i\hbar \frac{d}{dx}\psi_p = p\psi_p, \qquad (*)$$

where $\psi_p = \langle x|p\rangle$ is the wavefunction corresponding to the momentum eigenstate p. This equation can be integrated directly:

$$\frac{1}{\psi_p}\frac{d\psi_p}{dx} = \frac{ip}{\hbar}$$

$$\text{i.e.} \quad \int \frac{d\psi_p}{\psi_p} = \frac{ip}{\hbar}\int dx$$

$$\text{i.e.} \quad \ln\psi_p = \frac{ip}{\hbar}x + \text{const}$$

$$\text{or} \quad \psi_p = Ce^{ipx/\hbar}, \quad \text{as required.}$$

[NB. The equation "$-i\hbar\nabla|p\rangle = p|p\rangle$" is not correct: it is a mixture of the Dirac notation & the co-ordinate representation, & mathematically it is nonsense. To see this, consider the formal path from Eq. (1) to (*): take the inner product of (1) with $|x\rangle$:

$$\langle x|\hat{p}|p\rangle = p\langle x|p\rangle$$

$$\text{i.e.} \quad \int dx \langle x|\hat{p}|x'\rangle\langle x'|p\rangle = p\langle x|p\rangle$$

& then $\langle x|\hat{p}|x'\rangle = -i\hbar\,\delta(x-x')\frac{d}{dx} \Rightarrow$

$$-i\hbar\frac{d}{dx}\langle x|p\rangle = p\langle x|p\rangle$$

which is (*). Nowhere does "$-i\hbar\nabla|p\rangle = p|p\rangle$" appear!

Differentiating $e^{-ipx/\hbar}$ wrt p will bring out a factor $-ix/\hbar$, i.e.

$$\frac{d}{dp}\left(e^{-ipx/\hbar}\right) = \frac{-ix}{\hbar} e^{-ipx/\hbar}$$

or $$i\hbar \frac{d}{dp}\left(e^{-ipx/\hbar}\right) = x\, e^{-ipx/\hbar} \qquad (D2)$$

Comparing (D1) & (D2) we identify

$$\tilde{x} = i\hbar \frac{d}{dp}.$$

(e). Consider the action of the commutator (which is an operator) on an arbitrary wave function $\phi = \phi(p)$ in momentum space:

$$\begin{aligned}
[\tilde{x}, \tilde{p}]\,\phi &= (\tilde{x}\tilde{p} - \tilde{p}\tilde{x})\,\phi \\
&= i\hbar \frac{d}{dp}(p\phi) - p\, i\hbar \frac{d\phi}{dp} \\
&= i\hbar\left(\phi + \cancel{p\frac{d\phi}{dp}} - \cancel{p\frac{d\phi}{dp}}\right) \\
&= i\hbar\,\phi
\end{aligned}$$

which establishes $[\tilde{x}, \tilde{p}] = i\hbar$.

SOLUTION TO PHYS 304 QUANTUM PHYSICS II 2000 ASS. 6

1. The matrix elements for the momentum operator are

$$p_{nm} = \int_{-\infty}^{+\infty} \psi_n \tilde{p} \psi_m \, dx$$

$$= \int_{-\infty}^{+\infty} \psi_n \left(-i\hbar \frac{d}{dx}\right) \psi_m \, dx .$$

From lectures we have

$$\psi_n = v_n(\xi) \left|\frac{d\xi}{dx}\right|^{\frac{1}{2}}, \qquad \xi = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}} x ,$$

so

$$p_{nm} = -i\hbar \int_{-\infty}^{+\infty} v_n(\xi) \left|\frac{d\xi}{dx}\right|^{\frac{1}{2}} \frac{d\xi}{dx} \frac{d}{d\xi} \cdot v_m(\xi) \left|\frac{d\xi}{dx}\right|^{\frac{1}{2}} \frac{dx}{d\xi} \cdot d\xi$$

$$= -i\hbar \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}} \int_{-\infty}^{+\infty} v_n(\xi) \frac{d v_m(\xi)}{d\xi} \cdot d\xi \qquad (1)$$

Taking the difference of the recurrence relations for the SHO wavefunctions given in lectures we have

$$\left[\left(\xi + \frac{d}{d\xi}\right) - \left(\xi - \frac{d}{d\xi}\right)\right] v_m(\xi) = (2m)^{\frac{1}{2}} v_{m-1}(\xi) - \left[2(m+1)\right]^{\frac{1}{2}} v_{m+1}(\xi)$$

$$\text{i.e.} \quad 2 \frac{d v_m(\xi)}{d\xi} = (2m)^{\frac{1}{2}} v_{m-1}(\xi) - \left[2(m+1)\right]^{\frac{1}{2}} v_{m+1}(\xi)$$

$$\text{or} \quad \frac{d v_m(\xi)}{d\xi} = \frac{1}{\sqrt{2}} \left[m^{\frac{1}{2}} v_{m-1}(\xi) - (m+1)^{\frac{1}{2}} v_{m+1}(\xi) \right].$$

Substituting this into (1) gives

$$p_{nm} = -i\left(\frac{m\hbar\omega}{2}\right)^{\frac{1}{2}}\left[m^{\frac{1}{2}}\int_{-\infty}^{+\infty} v_n(\xi)\,v_{m-1}(\xi)\,d\xi - (m+1)^{\frac{1}{2}}\int_{-\infty}^{+\infty} v_n(\xi)\,v_{m+1}(\xi)\,d\xi\right]$$

$$2 \quad = -i\left(\frac{m\hbar\omega}{2}\right)^{\frac{1}{2}}\left[m^{\frac{1}{2}}\delta_{n,m-1} - (m+1)^{\frac{1}{2}}\delta_{n,m+1}\right]$$

using the orthonormality of the $v_n(\xi)$. In matrix form this is

$$p_{nm} = [\langle n|\hat{p}|m\rangle] = i\left(\frac{m\hbar\omega}{2}\right)^{\frac{1}{2}}\begin{pmatrix} 0 & -\sqrt{1} & 0 & 0 & \cdots \\ \sqrt{1} & 0 & -\sqrt{2} & 0 & \cdots \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix}$$

2

as required.

2. Eq. (1) shows that the matrix corresponding to $\hat{x}^2$ is the matrix for $\hat{x}$ times itself.

Hence:

$$[\hat{x}^2] = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}\cdot\left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}\cdot\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix}$$

2

(using the result for $[\hat{x}]$ from lectures)

$$= \left(\frac{\hbar}{2m\omega}\right)\cdot\begin{pmatrix} 1 & 0 & \sqrt{2} & 0 & \cdots \\ 0 & 3 & 0 & \sqrt{6} & \cdots \\ \sqrt{2} & 0 & 5 & 0 & \cdots \\ 0 & \sqrt{6} & 0 & 7 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix}$$

2

The appearance of the different values is made more obvious by rewriting this as

SOLUTION TO PHYS 304 QUANTUM PHYSICS II ASS. 7

1. (a). $\langle \hat{J}_z \rangle = m\hbar$ (the system is in an eigenstate of $\hat{J}_z$, so a measurement returns the eigenvalue)

$$\langle \hat{J}_x \rangle = \frac{1}{2}\langle \hat{J}_+ + \hat{J}_- \rangle$$

$$= \frac{1}{2}\langle jm | (\hat{J}_+ + \hat{J}_-) | jm \rangle$$

$$= \frac{1}{2}\langle jm | \hat{J}_+ | jm \rangle + \frac{1}{2}\langle jm | \hat{J}_- | jm \rangle$$

$$= \frac{1}{2} C_+(j,m) \langle jm | j\,m+1 \rangle + \frac{1}{2} C_-(j,m) \langle jm | j\,m-1 \rangle$$

$= 0$, since the states corresponding to different m's are orthogonal.

$$\langle \hat{J}_x^2 \rangle = \frac{1}{4}\langle (\hat{J}_+ + \hat{J}_-)^2 \rangle$$

$$= \frac{1}{4}\langle \hat{J}_+^2 + \hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+ + \hat{J}_-^2 \rangle$$

$$= \frac{1}{4}\langle jm | \hat{J}_+\hat{J}_- | jm \rangle + \frac{1}{4}\langle jm | \hat{J}_-\hat{J}_+ | jm \rangle$$

(the terms with $\hat{J}_+^2$ & $\hat{J}_-^2$ are zero because they will involve inner products of $|jm\rangle$ with $|j\,m+2\rangle$ & $|j\,m-2\rangle$, respectively).

So $\langle \hat{J}_x^2 \rangle = \frac{1}{4}\hbar\left[(j+m)(j-m+1)\right]^{\frac{1}{2}} \langle jm | \hat{J}_+ | j\,m-1 \rangle$

$$+ \frac{1}{4}\hbar\left[(j-m)(j+m+1)\right]^{\frac{1}{2}} \langle jm | \hat{J}_- | j\,m+1 \rangle$$

applying the rules for the actions of $\hat{J}_\pm$ once,

& $\langle \hat{J}_x^2 \rangle = \frac{1}{4}\hbar^2\left[(j+m)(j-m+1)\right]^{\frac{1}{2}}\left[(j-(m-1))(j+m-1+1)\right]^{\frac{1}{2}} \langle jm | jm \rangle$

$$+ \frac{1}{4}\hbar^2\left[(j-m)(j+m+1)\right]^{\frac{1}{2}}\left[(j+m+1)(j-(m+1)+1)\right] \langle jm | jm \rangle$$

$$[\hat{X}^2] = \frac{\hbar}{2m\omega}\begin{pmatrix} 1 & 0 & \sqrt{1\cdot 2} & 0 & \cdots \\ 0 & 1+2 & 0 & \sqrt{2\cdot 3} & \cdots \\ \sqrt{1\cdot 2} & 0 & 2+3 & 0 & \cdots \\ 0 & \sqrt{2\cdot 3} & 0 & 3+4 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix}$$

as the diagonal elements are the sums of consecutive integers, & the off-diagonal elements are the products of consecutive integers.

3. $[\hat{a}, \hat{a}^\dagger] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}$

$= \left(\frac{\hat{H}}{\hbar\omega} + \frac{1}{2}\right) - \left(\frac{\hat{H}}{\hbar\omega} - \frac{1}{2}\right)$, using (2)

$= 1$, as required. 2

consider

$\hat{a}\hat{H} = \hat{a}\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\hbar\omega$, using (2)

$= (\hat{a}\hat{a}^\dagger)\hat{a}\hbar\omega + \frac{1}{2}\hbar\omega\hat{a}$

$= \hbar\omega\left(\frac{\hat{H}}{\hbar\omega} + \frac{1}{2}\right)\hat{a} + \frac{1}{2}\hbar\omega\hat{a}$, using (2)

$= \hat{H}\hat{a} + \hbar\omega\hat{a}$ 2

& hence $[\hat{a}, \hat{H}] = \hbar\omega\hat{a}$, as required.

Finally

$\hat{a}^\dagger\hat{H} = \hat{a}^\dagger\left(\hat{a}\hat{a}^\dagger - \frac{1}{2}\right)\hbar\omega$, using (2)

$= (\hat{a}^\dagger\hat{a})\hat{a}^\dagger\hbar\omega - \frac{1}{2}\hbar\omega\hat{a}^\dagger$

$= \left(\frac{\hat{H}}{\hbar\omega} - \frac{1}{2}\right)\hat{a}^\dagger\hbar\omega - \frac{1}{2}\hbar\omega\hat{a}^\dagger$

$= \hat{H}\hat{a}^\dagger - \hbar\omega\hat{a}^\dagger$, hence $[\hat{a}^\dagger, \hat{H}] = -\hbar\omega\hat{a}^\dagger$, 2

as required.

where $n_{max,j}$ is the largest integer less than or equal to j.

(c). When the system is in an eigenstate of $\hat{J}_z$, all positive values for J_x are just as likely as negative values. Hence the average of many measurements will give zero. Another way of saying this is that there is no preferred orientation in the x-y plane for $\underset{\sim}{J}$.

As for $\langle J_x^2 \rangle$, the average of a set of positive numbers must be non-zero. It is also physically obvious that $\langle J_x^2 \rangle$ should increase with j (because $|\underset{\sim}{J}|$ is larger) & should be largest when $|m|$ is a minimum (the vector $\underset{\sim}{J}$ then has larger projections into the x-y plane).

2. (a). First construct the matrices for $\hat{J}_\pm$. We have:

$$\langle j m' | \hat{J}_+ | j m \rangle = \hbar \left[(j-m)(j+m+1) \right]^{\frac{1}{2}} \langle j m' | j m+1 \rangle$$

$$= \hbar \left[(j-m)(j+m+1) \right]^{\frac{1}{2}} \delta_{m' m+1}$$

or in matrix form,

$$\frac{1}{\hbar} \left[\hat{J}_+ \right] = \begin{array}{c} \\ m'=1 \\ 0 \\ -1 \end{array} \begin{array}{c} \begin{array}{ccc} \quad m=1 & \quad 0 & \quad -1 \end{array} \\ \begin{pmatrix} 0 & [(1-0)(1+1)]^{\frac{1}{2}} & 0 \\ 0 & 0 & [(1+1)(1-1+1)]^{\frac{1}{2}} \\ 0 & 0 & 0 \end{pmatrix} \end{array}$$

$$= \tfrac{1}{4}\hbar^2\left[(j+m)(j-m+1)+(j-m)(j+m+1)\right],$$

applying the rules again. Hence

$$\langle \hat{J}_x^2 \rangle = \tfrac{1}{4}\hbar^2\left[(j+m)(j-m+1+j-m)+j-m\right]$$

$$= \tfrac{1}{4}\hbar^2\left[(j+m)(2j-2m+1)+j-m\right]$$

$$= \tfrac{1}{4}\hbar^2\left[2j^2-\cancel{2mj}+j+\cancel{2mj}-2m^2+\cancel{m}+j-\cancel{m}\right]$$

$$= \tfrac{1}{4}\hbar^2\left[2j^2+2j-2m^2\right]$$

$$= \tfrac{1}{2}\hbar^2\left(j^2+j-m^2\right)$$

(b). The system is in an eigenstate of $\hat{J}_z$ so the only possible outcome of a measurement of the z-component of momentum is the eigenvalue, viz. $m\hbar$.

Measurement of the x-component of momentum will return one of the possible values

$$-j\hbar,\ -(j-1)\hbar,\ \ldots,\ (j-1)\hbar,\ j\hbar.$$

(These are the eigenvalues for any component of momentum. However, the system is not in an eigenstate of $\hat{J}_x$ & so it is not certain which eigenvalue will be observed.)

Measurement of the square of J_x will return one of the values

$$(-j\hbar)^2,\ [-(j-1)\hbar]^2,\ \ldots,\ [(j-1)\hbar]^2,\ (j\hbar)^2$$

i.e. $j^2\hbar^2,\ (j-1)^2\hbar^2,\ \ldots,\ (j-n_{max,j})^2\hbar^2,$

i.e. $[\hat{J}_+] = \hbar \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix}$.

Similarly

$$\langle jm'|\hat{J}_-|jm\rangle = \hbar[(j+m)(j-m+1)]^{\frac{1}{2}}\delta_{m'm-1}$$

so $\frac{1}{\hbar}[\hat{J}_-] =$

m' \ m	1	0	−1
1	0	0	0
0	$[(1+1)(1)]^{\frac{1}{2}}$	0	0
−1	0	$[(1+0)(1+1)]^{\frac{1}{2}}$	0

i.e. $[\hat{J}_-] = \hbar \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}$

Then we have $\hat{J}_x = \frac{1}{2}(\hat{J}_+ + \hat{J}_-)$, so

$$[\hat{J}_x] = \frac{1}{2}\hbar\left[\begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}\right]$$

$$= \frac{1}{2}\hbar \begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$

Similarly $\hat{J}_y = \frac{1}{2i}(\hat{J}_+ - \hat{J}_-)$, so

$$[\hat{J}_y] = \frac{1}{2i}\hbar\left[\begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}\right]$$

$$= \frac{-i}{2}\hbar \begin{pmatrix} 0 & \sqrt{2} & 0 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{pmatrix}.$$

Finally

$$\langle jm'|\hat{J}_z|jm\rangle = \hbar m\delta_{m'm}, \text{ so}$$

$$[\hat{J}_z] = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

(b). Dropping the [ ] notation we have

$$\hat{J}_x\hat{J}_y = -\frac{i}{4}\hbar^2\begin{pmatrix}0&\sqrt{2}&0\\ \sqrt{2}&0&\sqrt{2}\\ 0&\sqrt{2}&0\end{pmatrix}\begin{pmatrix}0&\sqrt{2}&0\\ -\sqrt{2}&0&\sqrt{2}\\ 0&-\sqrt{2}&0\end{pmatrix}$$

$$= -\frac{i}{4}\hbar^2\begin{pmatrix}-2&0&2\\ 0&0&0\\ -2&0&2\end{pmatrix}$$

$$= -\frac{i}{2}\hbar\begin{pmatrix}-1&0&1\\ 0&0&0\\ -1&0&1\end{pmatrix}$$

& $$\hat{J}_y\hat{J}_x = -\frac{i}{4}\hbar^2\begin{pmatrix}0&\sqrt{2}&0\\ -\sqrt{2}&0&\sqrt{2}\\ 0&-\sqrt{2}&0\end{pmatrix}\begin{pmatrix}0&\sqrt{2}&0\\ \sqrt{2}&0&\sqrt{2}\\ 0&\sqrt{2}&0\end{pmatrix}$$

$$= -\frac{i}{4}\hbar^2\begin{pmatrix}2&0&2\\ 0&0&0\\ -2&0&-2\end{pmatrix}$$

$$= -\frac{i}{2}\hbar^2\begin{pmatrix}1&0&1\\ 0&0&0\\ -1&0&-1\end{pmatrix}$$

So $$\hat{J}_x\hat{J}_y - \hat{J}_y\hat{J}_x = -\frac{i}{2}\hbar^2\left[\begin{pmatrix}-1&0&1\\ 0&0&0\\ -1&0&1\end{pmatrix} - \begin{pmatrix}1&0&1\\ 0&0&0\\ -1&0&-1\end{pmatrix}\right]$$

$$= -\frac{i}{2}\hbar^2\begin{pmatrix}-2&0&0\\ 0&0&0\\ 0&0&2\end{pmatrix}$$

$$= i\hbar\cdot\hbar\begin{pmatrix}1&0&0\\ 0&0&0\\ 0&0&-1\end{pmatrix}$$

$$= i\hbar\hat{J}_z.$$

Hence we have established that

$$[\hat{J}_x, \hat{J}_y] = i\hbar\hat{J}_z.$$

SOLUTION TO PHYS 304 QUANTUM PHYS. II ASS. 8

1. $[\hat{J}_x, \hat{J}_y] = [\hat{J}_{1x} + \hat{J}_{2x}, \hat{J}_{1y} + \hat{J}_{2y}]$

$= [\hat{J}_{1x}, \hat{J}_{1y}] + \cancel{[\hat{J}_{1x}, \hat{J}_{2y}]}$

$+ \cancel{[\hat{J}_{2x}, \hat{J}_{1y}]} + [\hat{J}_{2x}, \hat{J}_{2y}]$

(because $[\hat{J}_{1i}, \hat{J}_{2j}] = 0, \quad i,j = x,y,z$),

i.e. $[\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_{1z} + i\hbar \hat{J}_{2z}$

(since $\underset{\sim}{J}_1$ & $\underset{\sim}{J}_2$ are angular momenta),

i.e. $[\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z$, as required.

The others proceed similarly:

$[\hat{J}_y, \hat{J}_z] = [\hat{J}_{1y} + \hat{J}_{2y}, \hat{J}_{1z} + \hat{J}_{2z}]$

$= [\hat{J}_{1y}, \hat{J}_{1z}] + \cancel{[\hat{J}_{1y}, \hat{J}_{2z}]}$

$+ \cancel{[\hat{J}_{2y}, \hat{J}_{1z}]} + [\hat{J}_{2y}, \hat{J}_{2z}]$

$= i\hbar \hat{J}_{1x} + i\hbar \hat{J}_{2x} = i\hbar \hat{J}_x,$

& $[\hat{J}_z, \hat{J}_x] = [\hat{J}_{1z} + \hat{J}_{2z}, \hat{J}_{1x} + \hat{J}_{2x}]$

$= [\hat{J}_{1z}, \hat{J}_{1x}] + \cancel{[\hat{J}_{1z}, \hat{J}_{2x}]}$

$+ \cancel{[\hat{J}_{2z}, \hat{J}_{1x}]} + [\hat{J}_{2z}, \hat{J}_{2x}]$

$= i\hbar \hat{J}_{1y} + i\hbar \hat{J}_{2y} = i\hbar \hat{J}_y,$

as required.

2. $(\underset{\sim}{\sigma}\cdot\underset{\sim}{A})(\underset{\sim}{\sigma}\cdot\underset{\sim}{B})$

$$= (\sigma_x A_x + \sigma_y A_y + \sigma_z A_z)(\sigma_x B_x + \sigma_y B_y + \sigma_z B_z)$$

$$= \sigma_x^2 A_x B_x + \sigma_y^2 A_y B_y + \sigma_z^2 A_z B_z$$

$$+ \sigma_x\sigma_y A_x B_y + \sigma_x\sigma_z A_x B_z + \sigma_y\sigma_x A_y B_x$$

$$+ \sigma_y\sigma_z A_y B_z + \sigma_z\sigma_x A_z B_x + \sigma_z\sigma_y A_z B_y$$

$$= I A_x B_x + I A_y B_y + I A_z B_z$$

$$+ i\sigma_z A_x B_y \quad -i\sigma_y A_x B_z \quad -i\sigma_z A_y B_x$$

$$+ i\sigma_x A_y B_z \quad +i\sigma_y A_z B_x \quad -i\sigma_x A_z B_y$$

(using the properties of the Pauli matrices)

$$= I(\underset{\sim}{A}\cdot\underset{\sim}{B}) + i\sigma_x(A_y B_z - A_z B_y)$$

$$+ i\sigma_y(A_z B_x - A_x B_z) + i\sigma_z(A_x B_y - A_y B_x).$$

Noting that

$$\underset{\sim}{A}\times\underset{\sim}{B} = \begin{vmatrix} \hat{\underset{\sim}{x}} & \hat{\underset{\sim}{y}} & \hat{\underset{\sim}{z}} \\ A_x & A_y & A_z \\ B_x & B_y & B_z \end{vmatrix} = [A_y B_z - A_z B_y,\ A_z B_x - A_x B_z,\ A_x B_y - A_y B_x]$$

we have established

$$(\underset{\sim}{\sigma}\cdot\underset{\sim}{A})(\underset{\sim}{\sigma}\cdot\underset{\sim}{B}) = I(\underset{\sim}{A}\cdot\underset{\sim}{B}) + i\underset{\sim}{\sigma}\cdot(\underset{\sim}{A}\times\underset{\sim}{B}),$$

as required.

3. $\langle \hat{\underset{\sim}{J}} \cdot \hat{\underset{\sim}{a}} \rangle = \langle \tfrac{1}{2}\tfrac{1}{2} | \{ \hat{J}_z \cos\phi + \frac{1}{2i}(\hat{J}_+ - \hat{J}_-) \sin\phi \} | \tfrac{1}{2}\tfrac{1}{2} \rangle$

$= \langle \tfrac{1}{2}\tfrac{1}{2} | \hat{J}_z | \tfrac{1}{2}\tfrac{1}{2} \rangle \cos\phi$

(since $\hat{J}_+ | \tfrac{1}{2}\tfrac{1}{2} \rangle = \langle \tfrac{1}{2}\tfrac{1}{2} | \hat{J}_- | \tfrac{1}{2}\tfrac{1}{2} \rangle = 0$)

$= \frac{1}{2}\hbar \cos\phi = \frac{1}{2}\hbar \left(\cos^2\frac{\phi}{2} - \sin^2\frac{\phi}{2} \right)$,

as found in lectures.

MACQUARIE
UNIVERSITY~SYDNEY

End of Year Examination 2000

Unit:	PHYS304–QUANTUM PHYSICS
Date and Time:	28 November 2000 9:20am
Time Allowed:	THREE (3) hours, plus 10 minutes reading time.
Total Number of Questions:	Eight (8)
Instructions:	Answer FIVE (5) questions, at least TWO (2) from each of Sections A and B Answer Sections A and B in separate books. The questions are of equal value. Calculators may be used except for those having a full alphabet on the keyboard.

The following information may be useful:

All vectors in ordinary space are in **bold type**, e.g. **A**, **r**.

All operators are indicated by a "$\frown$", e.g. $\widehat{A}$, $\widehat{\mathbf{r}}$.

All operators in the position representation are indicated by a "$\sim$", e.g. $\widetilde{p}$.

QUESTION A2

(a) (3 marks)

The ket vectors $\{|\varphi_n\rangle; n = 1, 2, \ldots\}$ form a complete, orthonormal set of basis states. Explain what the terms "complete", "orthonormal", and "basis" mean.

(b) (4 marks)

One of the following ket vectors is not a physically permissible state. Which one is acceptable, and explain why.

$$|\phi\rangle = \sum_{n=0}^{\infty} \frac{1}{\sqrt{n+1}} |\varphi_n\rangle; \quad |\psi\rangle = \sum_{n=0}^{\infty} \frac{1}{n+1} |\varphi_n\rangle$$

(c) (7 marks)

State whether each of the following statements is true or false, and if false, either write down the correct statement or explain why the statement is false.

(i) For any operator $\widehat{A}$, if $\widehat{A}|\psi\rangle = |\phi\rangle$, then $\langle\psi|\widehat{A} = \langle\phi|$.

(ii) The ket vectors $|\psi\rangle$ and $e^{i\phi}|\psi\rangle$ represent different physical states of a system.

(iii) If $\widehat{A}$ is a linear operator, then $\widehat{A}\big(|\psi\rangle + |\phi\rangle\big) = \widehat{A}|\psi\rangle + \widehat{A}|\phi\rangle$.

(iv) If $\widehat{A} = \widehat{A}^\dagger$ then $\widehat{A}$ has real eigenvalues.

(v) If $\widehat{A}\widehat{A}^\dagger = \widehat{A}^\dagger\widehat{A} = \widehat{1}$ then $\widehat{A}$ is Hermitean.

(vi) The state $|\psi\rangle \doteq \begin{pmatrix} 2 \\ i \end{pmatrix}$ is normalized to unity.

(vii) $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^*$

(d) (6 marks)

If $\widehat{A}$ is a Hermitean operator with eigenstates $\{|a_n\rangle; n = 1, 2, \ldots\}$ and associated eigenvalues $a_n, n = 1, 2, \ldots$, show that

$$\langle\psi|f(\widehat{A})|\psi\rangle = \sum_n f(a_n)|\langle\psi|a_n\rangle|^2$$

where $f(x)$ is a function that can be expanded as a power series in x.

QUESTION A4

(a) (8 marks)

State, without proof, what the mathematical and physical significance is of two observables $\widehat{A}$ and $\widehat{B}$ (i) commuting, (ii) not commuting. Your answer should include comments concerning the link between the commutation relation between two observables and the uncertainty principle.

(b) (8 marks)

The space displacement operator $\widehat{\mathcal{D}}(a)$ is defined such that $\widehat{\mathcal{D}}(a)|x\rangle = |x+a\rangle$, and can be shown to be given by $\widehat{\mathcal{D}}(a) = e^{i\widehat{p}a/\hbar}$.

(i) Show that $[\widehat{x}, \widehat{p}] = i\hbar$.

(ii) Show that $\widehat{p}$ is a Hermitean operator.

(iii) What observable can $\widehat{p}$ be identified with?

(c) (4 marks)

Describe briefly the procedure of canonical quantisation for a system consisting of a single particle moving in one dimension under the action of a potential.

QUESTION B2

(a) (7 marks)

The solution to the Schrödinger equation for the simple harmonic oscillator (SHO) is facilitated by introducing the variable

$$\xi = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}} x,$$

and by introducing the wavefunctions in this variable, $v_n(\xi)$, which are normalised according to

$$|\psi_n(x)|^2 dx = |v_n(\xi)|^2 d\xi.$$

The new wavefunctions satisfy the recurrence relations

$$\begin{aligned} \frac{1}{\sqrt{2}}\left(\xi + \frac{d}{d\xi}\right) v_n(\xi) &= n^{\frac{1}{2}} v_{n-1}(\xi), \\ \frac{1}{\sqrt{2}}\left(\xi - \frac{d}{d\xi}\right) v_n(\xi) &= (n+1)^{\frac{1}{2}} v_{n+1}(\xi). \end{aligned}$$

Use these results to determine the matrix elements for the position operator for the SHO,

$$x_{nm} = \int_{-\infty}^{+\infty} \psi_n(x) x \psi_m(x)\, dx.$$

(b) (3 marks)

Construct the matrix corresponding to the elements x_{nm}.

(c) (4 marks)

What is $\langle x \rangle$ when the SHO is in an energy eigenstate? Give a physical reason for this result.

(d) (6 marks)

The recurrence relations above provide the co-ordinate representation of raising and lowering operators $\hat{a}^\dagger$ and $\hat{a}$ for the SHO. The general definition of these operators is

$$\hat{a} = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{x} + i\hat{p}) \qquad \hat{a}^\dagger = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{x} - i\hat{p})$$

and their action is

$$\hat{a}|n\rangle = n^{\frac{1}{2}}|n-1\rangle; \qquad \hat{a}^\dagger|n\rangle = (n+1)^{\frac{1}{2}}|n+1\rangle,$$

where $|n\rangle$ is the nth energy eigenstate for the SHO. Express $\hat{x}$ in terms of $\hat{a}$ and $\hat{a}^\dagger$ and use this result to determine $\langle n|\hat{x}|m\rangle$, i.e. the matrix elements for the position operator for the SHO. Show that the results are the same as (a).

QUESTION B4

(a) (4 marks)

Consider a system consisting of two identical particles. Summarise the argument that the system is described by a state that is either symmetric or antisymmetric under interchange of the particles.

(b) (3 marks)

Let $\psi(q_1, q_2)$ be an unsymmetrised wavefunction describing a system of two identical particles, where q_1 and q_2 denote the co-ordinates and spin states of the particles. If the particles are Fermions, construct an appropriately symmetrised wavefunction to describe the system. If the particles are Bosons, construct an appropriately symmetrised wavefunction to describe the system.

(c) (3 marks)

Summarise the argument that two identical spin $\frac{1}{2}$ particles have four possible spin states, three being symmetric and one antisymmetric.

(d) (4 marks)

The creation and annihilation operators for multiple-particle states of a system of identical weakly interacting Bosons are defined by

$$\begin{aligned} \widehat{a}_k|n_1, n_2, ..., n_k, ...\rangle &= n_k^{\frac{1}{2}}|n_1, n_2, ..., n_k - 1, ...\rangle, \\ \widehat{a}_k^\dagger|n_1, n_2, ..., n_k, ...\rangle &= (n_k + 1)^{\frac{1}{2}}|n_1, n_2, ..., n_k + 1, ...\rangle. \end{aligned}$$

Confirm that these operators satisfy the commutation relation $[\widehat{a}_k, \widehat{a}_l^\dagger] = \delta_{kl}$.

(e) (2 marks)

Explain why the operator $\widehat{N}_k = \widehat{a}_k^\dagger \widehat{a}_k$ is the "number operator."

(f) (4 marks)

The creation and annihilation operators for a system of identical weakly interacting Fermions satisfy a set of anticommutation relations,

$$\widehat{c}_k\widehat{c}_l + \widehat{c}_l\widehat{c}_k = 0, \quad \widehat{c}_k^\dagger\widehat{c}_l^\dagger + \widehat{c}_l^\dagger\widehat{c}_k^\dagger = 0, \quad \widehat{c}_k\widehat{c}_l^\dagger + \widehat{c}_l^\dagger\widehat{c}_k = \delta_{kl}.$$

Use these relations to show that the number operator ($\widehat{N}_k = \widehat{c}_k^\dagger\widehat{c}_k$) obeys $\widehat{N}_k^2 = \widehat{N}_k$.

Hence determine the possible values of the n_k. What principle does this represent?

ANSWERS + MARKING SCHEME

Q1. (a). The wavefunction is defined ~~to be~~ as the probability amplitude for being at the position $\underset{\sim}{x}$ given the particle is in the state $|\psi\rangle$, i.e. (3)

$$\psi(\underset{\sim}{x},t) = \langle \underset{\sim}{x} | \psi \rangle \quad (1)$$

in the usual notation, where $|\psi\rangle$ is the state vector for the system & $|\underset{\sim}{x}\rangle$ is a position basis state corresponding to $\underset{\sim}{x}$. (1)

The physical interpretation of the wavefunction is that

$$|\psi(\underset{\sim}{x},t)|^2 d^3\underset{\sim}{x} \quad (1)$$

is the probability for finding the particle in the infinitesimal volume $dV = d^3\underset{\sim}{x}$ about $\underset{\sim}{x}$ at time t, i.e. for finding the particle in the cube defined by $x+dx$, $y+dy$ & $z+dz$ where $d^3\underset{\sim}{x} = dx\,dy\,dz$.

(b). We have (4)

$$I = \int_{-\infty}^{+\infty} \chi^* \left(-i\hbar \frac{d\psi}{dx}\right) dx$$

$$= \left[-i\hbar \chi^* \psi\right]_{-\infty}^{\infty} - \int_{-\infty}^{+\infty} (-i\hbar)\,\psi \frac{d\chi^*}{dx}\,dx \quad (1)$$

$$= 0 \quad (1) \quad - \int_{-\infty}^{+\infty} (-i\hbar)\,\psi \frac{d\chi^*}{dx}\,dx \quad (1)$$

since the wavefunctions go to zero as $x \to \pm\infty$.

Hence

$$I = \int_{-\infty}^{+\infty} \psi \, i\hbar \frac{d\chi^*}{dx} \, dx$$

$$= \left[\int_{-\infty}^{+\infty} \psi^* \left(-i\hbar \frac{d\chi}{dx} \right) dx \right]^* \quad (1)$$

as required.

(c). We have

(2)
$$\int_{-\infty}^{+\infty} \chi^* \left(-i\hbar \frac{d}{dx} \psi \right) dx = \left[\int_{-\infty}^{+\infty} \psi^* \left(-i\hbar \frac{d}{dx} \chi \right) dx \right]^*$$

&
$$\langle \chi | \hat{Q} | \psi \rangle = \langle \psi | \hat{Q}^\dagger | \chi \rangle^*$$

From lectures we know

$$\langle \psi | \hat{Q}^\dagger | \chi \rangle \rightarrow \int_{-\infty}^{+\infty} \psi^* \tilde{Q}^\dagger \chi \, dx \quad (1)$$

in the co-ordinate representation & hence we identify

$$\tilde{p}^\dagger = -i\hbar \frac{d}{dx} \quad (1)$$

as the Hermitian conjugate of the momentum operator in the co-ordinate representation.

(d). The operators $\hat{Q}$ corresponding (2) to any physical observable must be Hermitian (1), ~~(i.e. their Hermitian conjugate is the~~

i.e.

$$\hat{Q}^\dagger = \hat{Q} \quad (1)$$

Hence the result in (c) was expected.

(e). The position operator in the (4) co-ordinate representation is the position vector (i.e. the action of the operator is multiplication by the position vector). In 1-D

$$\tilde{x} = x \quad (1)$$

The basic commutation relation is

$$[\tilde{p}, \tilde{x}] = -i\hbar \quad (1) \qquad [\tilde{x}, \tilde{p}] = i\hbar$$

To see that it satisfied, consider the operation of the LHS on an arbitrary wavefn ψ:

$$[\tilde{p}, \tilde{x}]\psi = (\tilde{p}\tilde{x} - \tilde{x}\tilde{p})\psi \quad (1)$$

$$= \left[-i\hbar \frac{d}{dx} x - x\left(-i\hbar \frac{d}{dx}\right)\right]\psi$$

$$= -i\hbar \frac{d}{dx}(x\psi) + i\hbar x \frac{d\psi}{dx}$$

$$= -i\hbar x \frac{d\psi}{dx} - i\hbar\psi + i\hbar x \frac{d\psi}{dx} = -i\hbar\psi \quad (1)$$

(f). (3)

$$-i\hbar \frac{d\psi_p}{dx} = p\psi_p \quad (\text{i.e. } \tilde{p}\psi_p = p\psi_p) \qquad ① ①$$

$$\text{so} \quad -\frac{1}{\psi_p}\frac{d\psi_p}{dx} = -\frac{ip}{\hbar}$$

$$\Rightarrow \boxed{\psi_p = C e^{ipx/\hbar}} \quad ①$$

(g). (2)

$$\langle x \rangle = \int_{-\infty}^{+\infty} \psi_p^* x \psi_p \, dx$$

$$= |C|^2 \int_{-\infty}^{+\infty} x \, dx = \infty \quad ①$$

So there is no expectation value for position: all values are equally likely & the average is undefined. Since according to the uncertainty principle x must be unknown. Hence

① 15min?

22.

(a): $x_{nm} = \int_{-\infty}^{+\infty} \psi_n \, x \, \psi_m \, dx$ (7)

$=$

$$\psi_n = v_n \left(\frac{d\xi}{dx}\right)^{\frac{1}{2}} = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{4}} v_n$$ (1)

1 1 2 1

so: $x_{nm} = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}} \int_{-\infty}^{+\infty} v_n \left(\frac{\hbar}{m\omega}\right)^{\frac{1}{2}} \xi \, v_m \frac{dx}{d\xi} \, d\xi$ (2)

$= \left(\frac{\hbar}{m\omega}\right)^{\frac{1}{2}} \int_{-\infty}^{+\infty} v_n \, \xi \, v_m \, d\xi$ (2) (4)

& then adding the recurrence relations:

$$\frac{2}{\sqrt{2}} \xi v_n = n^{\frac{1}{2}} v_{n-1} + (n+1)^{\frac{1}{2}} v_{n+1}$$ (1)

$$\xi v_n = \frac{1}{\sqrt{2}} \left(n^{\frac{1}{2}} v_{n-1} + (n+1)^{\frac{1}{2}} v_{n+1} \right)$$

so $x_{nm} = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}} \left[n^{\frac{1}{2}} \int_{-\infty}^{+\infty} v_n v_{m-1} \, d\xi \right.$

$\left. + (n+1)^{\frac{1}{2}} \int_{-\infty}^{+\infty} v_n v_{m+1} \, d\xi \right]$

(1)

$$x_{nm} = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}} \left[m^{\frac{1}{2}} \delta_{n,m-1} + (m+1)^{\frac{1}{2}} \delta_{n,m+1} \right]$$ (1)

since $$\int_{-\infty}^{+\infty} \psi_n \psi_m d\xi = \delta_{nm}$$ (2)

(b). (3)

$$\left(\frac{2m\omega}{\hbar}\right)^{\frac{1}{2}} [x_{nm}] = \begin{array}{c} n \\ \downarrow \\ \begin{matrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ \vdots \end{matrix} \end{array} \begin{array}{c} \begin{matrix} 0 & 1 & 2 & 3 & 4 & \cdots \end{matrix} \rightarrow m \\ \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \end{pmatrix} \end{array}$$ (3)

(c). (4)

$$\langle x \rangle = \langle n | \hat{x} | n \rangle$$ (1)

when the SHO is in an energy eigenstate so $\langle x \rangle = 0$ (1) (diagonal elements of matrix are zero) (1). Physically these are stationary states & because of the symmetry of the potential there is no reason for the particle to prefer to be in $x > 0$ or $x < 0$. (1)

~~Alternati~~

18

(d).

(6) $\langle n|\hat{x}|m\rangle = \quad ?$

$$\hat{a} = (2\hbar m\omega)^{-\frac{1}{2}}(m\omega\hat{x} + i\hat{p})$$

$$\hat{a}^\dagger = (\quad)^{-\frac{1}{2}}(m\omega\hat{x} - i\hat{p})$$

$$\hat{a} + \hat{a}^\dagger = \frac{1}{(2\hbar m\omega)^{\frac{1}{2}}}\, 2m\omega\hat{x} = \left(\frac{2m\omega}{\hbar}\right)^{\frac{1}{2}}\hat{x}$$

so $\hat{x} = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}(\hat{a} + \hat{a}^\dagger)$ (2)

so $\langle n|\hat{x}|m\rangle = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}\langle n|\hat{a} + \hat{a}^\dagger|m\rangle$

$$= \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}\Big\{m^{\frac{1}{2}}\langle n|m-1\rangle \quad (2)$$

$$+ (m+1)^{\frac{1}{2}}\langle n|m+1\rangle\Big\} \quad (2)$$

using the action of the operators

so $\langle n|\hat{x}|m\rangle = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}\Big[m^{\frac{1}{2}}\delta_{n\,m-1} + (m+1)^{\frac{1}{2}}\delta_{n\,m+1}\Big\}$ (2)

which is the same as in (a).

18 mins

Q3. (a). The definition of the orbital AM operator $\hat{\underset{\sim}{L}}$ is

(3)

$$\hat{\underset{\sim}{L}} = \hat{\underset{\sim}{x}} \times \hat{\underset{\sim}{p}} \quad (1)$$

where $\hat{\underset{\sim}{x}}$ & $\hat{\underset{\sim}{p}}$ are the position & momentum operators. In the co-ordinate representation we have

$$\hat{\underset{\sim}{L}} \to \tilde{\underset{\sim}{L}} = -i\hbar \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ x & y & z \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \end{vmatrix}$$

$$= -i\hbar \left[y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}, \; z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}, \; x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \right]$$

so

$$\tilde{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \right) \quad (2)$$

$$\tilde{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \right)$$

$$\tilde{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \right)$$

(b). $\langle J_z \rangle = \hbar m$ (the system is in an eigenstate with eigenvalue $\hbar m$)

(5)

$$\langle \hat{J}_x^2 \rangle = \frac{1}{4} \langle jm | (\hat{J}_+ + \hat{J}_-)^2 | jm \rangle$$

$$= \frac{1}{4}\langle jm | \hat{J}_+^2 + \hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+ + \hat{J}_-^2 | jm\rangle$$

$$= \frac{1}{4}\langle jm | \hat{J}_+\hat{J}_- | jm\rangle + \frac{1}{4}\langle jm | \hat{J}_-\hat{J}_+ | jm\rangle$$

$$= \frac{1}{4}\hbar\left[(j+m)(j-m+1)\right]^{\frac{1}{2}}\langle jm | \hat{J}_+ | j\,m-1\rangle$$

$$+ \frac{1}{4}\hbar\left[(j-m)(j+m+1)\right]^{\frac{1}{2}}\langle jm | \hat{J}_- | j\,m+1\rangle$$

$$= \frac{1}{4}\hbar^2\left[(j+m)(j-m+1)\right]^{\frac{1}{2}}\left[(j-m+1)(j+m)\right]^{\frac{1}{2}}\langle jm | jm\rangle$$

$$+ \frac{1}{4}\hbar^2\left[(j-m)(j+m+1)\right]^{\frac{1}{2}}\left[(j+m+1)(j-m)\right]^{\frac{1}{2}}\langle jm | jm\rangle$$

$$= \frac{1}{4}\hbar^2\left[(j+m)(j-m+1) + (j-m)(j+m+1)\right]$$

$$= \frac{1}{4}\hbar^2\left[(j+m)(j-m+1+j-m) + j-m\right]$$

$$= \frac{1}{4}\hbar^2\left[(j+m)(2j-2m+1) + j-m\right]$$

$$= \frac{1}{4}\hbar^2\left[2j^2 - 2mj + j + 2mj - 2m^2 + m + j - mj\right]$$

$$= \frac{1}{4}\hbar^2\left[2j^2 + 2j - 2m^2\right]$$

$$= \frac{1}{2}\hbar^2(j^2 + j - m^2) \quad (4)$$

Finally,

$$\langle \hat{J}^2 - \hat{J}_x^2 - \hat{J}_y^2\rangle = \langle \hat{J}_z^2\rangle = \hbar^2 m^2 \quad (1)$$

(c). measuring J_z: $\hbar m$ is the only possible outcome (1/2)

(3) " J_x^2: can get ~~m~~ any one of $(-\hbar j)^2$, $(-\hbar(j-1))^2$, ...

(1/2) , $\hbar^2(j-1)^2$, $\hbar^2 j^2$

(d). $|\frac{1}{2}\ \frac{1}{2}\rangle \rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

(5) $|\frac{1}{2}\ -\frac{1}{2}\rangle \rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$$\hat{J}_x = \frac{1}{2}(\hat{J}_+ + \hat{J}_-)$$

& $$\hat{J}_y = \frac{1}{2i}(\hat{J}_+ - \hat{J}_-)$$

so derive $\hat{J}_+$ first:

$$\langle j'm'|\hat{J}_+|jm\rangle$$

$$= \hbar\left[(j-m)(j+m+1)\right]^{\frac{1}{2}}\langle j'm'|j'm+1\rangle$$

$$= \hbar\left[(j-m)(j+m+1)\right]^{\frac{1}{2}}\delta_{m'm+1} \quad (j=j'=\tfrac{1}{2})$$

$$= \hbar\left[(\tfrac{1}{2}-m)(\tfrac{1}{2}+m+1)\right]^{\frac{1}{2}}\delta_{m'm+1}$$

(1)

so $$\left[\hat{J}_+\right] = \begin{matrix} \\ m' \downarrow \end{matrix}\begin{matrix} \overset{m}{\overset{\frac{1}{2}}{\longrightarrow}}\ \overset{}{-\frac{1}{2}} \\ \end{matrix}$$

$$\begin{matrix} \frac{1}{2} \\ -\frac{1}{2} \end{matrix}\begin{pmatrix} 0 & [1.1]^{\frac{1}{2}} \\ 0 & 0 \end{pmatrix} = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$\langle j'm' | \hat{J}_- | jm \rangle = \hbar \left[\left(\tfrac{1}{2}+m\right)\left(\tfrac{1}{2}-m+1\right) \right]^{\frac{1}{2}} \delta_{m'm-1}$$

$$\text{so} \quad [\hat{J}_-] = \begin{array}{c} \\ m'=\frac{1}{2} \\ m'=-\frac{1}{2} \end{array} \begin{array}{c} \begin{array}{cc} m=\frac{1}{2} & m=-\frac{1}{2} \end{array} \\ \hbar \begin{pmatrix} 0 & 0 \\ \sqrt{1} & 0 \end{pmatrix} \end{array}$$

$$= \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad (1)$$

$$\text{Hence} \quad \hat{J}_x = \tfrac{1}{2}(\hat{J}_+ + \hat{J}_-)$$

$$= \tfrac{1}{2}\hbar \left[\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \right]$$

$$= \tfrac{1}{2}\hbar \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (1)$$

$$\hat{J}_y = \frac{1}{2i}(\hat{J}_+ - \hat{J}_-)$$

$$[\hat{J}_y] = \frac{1}{2i}\hbar \left[\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \right]$$

$$= \frac{\hbar}{2i} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

$$= \tfrac{1}{2}\hbar \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (1)$$

$$\& \quad [\hat{J}_z] = \hbar \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix} = \tfrac{1}{2}\hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (1)$$

$$[\hat{J}_x][\hat{J}_y] = \left(\frac{1}{2}\hbar\right)^2 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

(4)

$$= \frac{\hbar^2}{4}\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$$ (1)

$$\& \quad [\hat{J}_y][\hat{J}_x] = \frac{\hbar^2}{4}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$= \frac{\hbar^2}{4}\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$$ (1)

$$\text{So} \quad [\hat{J}_x][\hat{J}_y] - [\hat{J}_y][\hat{J}_x] = \frac{\hbar^2}{4}\left[\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} - \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}\right]$$

$$= \frac{\hbar^2}{4}\begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix}$$

$$= \frac{\hbar^2}{2} i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$= \hbar i \cdot \frac{1}{2}\hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$= i\hbar [\hat{J}_z]$$ (1)

Hence we have established the matrices representing J_x, J_y & J_z satisfy $[\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z$. (1)

16 min.

4. (a). Introduce a permutation operator $\hat{P}_{12}$ (2) that interchanges the roles of the two identical particles (i.e. interchanges all attributes). If $|\Psi\rangle$ denotes an eigenstate of this operator, then (4)

$$\hat{P}_{12}|\Psi\rangle = \eta|\Psi\rangle \quad (1)$$

where η is the eigenvalue. But

$$\hat{P}_{12}^2|\Psi\rangle = \eta^2|\Psi\rangle = |\Psi\rangle, \quad (1)$$

since interchanging roles twice returns the original state of the system.

Hence $\eta^2 = 1 \Rightarrow \eta = \pm 1$ (1)

Hence the system is symmetric or antisymmetric under interchange of particles.

(b). The appropriate symmetrised wavefunction for (3) fermions is

$$\psi_a(q_1, q_2) = \frac{1}{\sqrt{2}}\left[\psi(q_1, q_2) - \psi(q_2, q_1)\right] \quad (1\tfrac{1}{2})$$

& for Bosons

$$\psi_s(q_1, q_2) = \frac{1}{\sqrt{2}}\left[\psi(q_1, q_2) + \psi(q_2, q_1)\right]. \quad (1\tfrac{1}{2})$$

these wavefunctions are antisymmetric & symmetric respectively, as required.

(c). Each particle (numbered 1, 2) can have spin up (denote α) or down (β) with respect to some axis. The possible combinations are

(3)

(1) $\alpha(1)\beta(2)$ $\alpha(2)\beta(1)$ $\alpha(2)\alpha(1)$ $\beta(2)\beta(1)$

The symmetric / antisymmetric combinations of these are:

SYMMETRIC	ANTISYMMETRIC
(1) $\alpha(1)\alpha(2)$	(1) $\frac{1}{\sqrt{2}}[\alpha(1)\beta(2) - \beta(1)\alpha(2)]$
$\beta(1)\beta(2)$	
$\frac{1}{\sqrt{2}}[\alpha(1)\beta(2) + \beta(1)\alpha(2)]$	

Hence there are four possible symmetrised spin states, three being symmetric & one antisymmetric.

(d). Consider two cases:

(4)

I. $k \neq \ell$. Then

$$\hat{a}_k \hat{a}_\ell^\dagger \,|n_1, n_2, \ldots, n_k, \ldots, n_\ell, \ldots\rangle$$

$$= (n_\ell + 1)^{\frac{1}{2}} \hat{a}_k \,|n_1, n_2, \ldots, n_k, \ldots, n_\ell + 1, \ldots\rangle$$

$$= (n_\ell + 1)^{\frac{1}{2}} (n_k)^{\frac{1}{2}} \,|n_1, n_2, \ldots, n_k - 1, \ldots, n_\ell + 1, \ldots\rangle$$

$= C_{nk}^{\dagger} C_{nl+1}$

$= n_k^{\frac{1}{2}} \hat{a} \hat{a}_l^{\dagger} \mid n_1, n_2, \ldots, n_k - 1, \ldots, n_l, \ldots \rangle$

$= \hat{a} \hat{a}_l^{\dagger} \hat{a}_k \mid n_1, n_2, \ldots, n_k, \ldots, n_l, \ldots \rangle$

So $\hat{a}_k \hat{a}_l^{\dagger} = \hat{a}_l^{\dagger} \hat{a}_k \Rightarrow [\hat{a}_k, \hat{a}_l^{\dagger}] = 0$ for $k \neq l$ (2)

<u>for $k = l$</u> (case II)

$\hat{a}_k \hat{a}_k^{\dagger} \mid n_1, n_2, \ldots, n_k, \ldots \rangle$

$= \hat{a}_k (n_k + 1)^{\frac{1}{2}} \mid n_1, n_2, \ldots, n_k + 1, \ldots \rangle$

$= (n_k + 1) \mid n_1, n_2, \ldots, n_k, \ldots \rangle$

& $\hat{a}_k^{\dagger} \hat{a}_k \mid n_1, n_2, \ldots, n_k, \ldots \rangle$

$= \hat{a}_k^{\dagger} n_k^{\frac{1}{2}} \mid n_1, n_2, \ldots, n_k - 1, \ldots \rangle$

$= n_k \mid n_1, n_2, \ldots, n_k, \ldots \rangle$

So $(\hat{a}_k \hat{a}_k^{\dagger} - \hat{a}_k^{\dagger} a_k) \mid n_1, n_2, \ldots, n_k, \ldots \rangle$

$= (n_k + 1 - n_k) \mid n_1, n_2, \ldots, n_k, \ldots \rangle$

$= \mid n_1, n_2, \ldots, n_k, \ldots \rangle$

& Hence $[\hat{a}_k^{\dagger}, \hat{a}_k] = 1$ (2)

Together these cases reestablish the commutator relation

$$[\hat{a}_k^\dagger \hat{a}_l] = \delta_{kl}.$$

(c). $\hat{N}_k |n_1, n_2, \ldots, n_k, \ldots\rangle$ (1)

(2) $= \hat{a}_k^\dagger \hat{a}_k |n_1 n_2, \ldots, n_k, \ldots\rangle$

$= \hat{a}_k^\dagger n_k^{\frac{1}{2}} |n_1, n_2, \ldots, n_k+1, \ldots\rangle$

$= n_k^{\frac{1}{2}} n_k^{\frac{1}{2}} |n_1, n_2, \ldots, n_k, \ldots\rangle$

$= n_k |n_1, n_2, \ldots, n_k, \ldots\rangle$ *

Hence $\hat{N}_k$ measures the number of particles in state k. (1)

(f). $\hat{N}_k^2 = \hat{c}_k^\dagger \hat{c}_k \hat{c}_k^\dagger \hat{c}_k$

(4) $= \hat{c}_k^\dagger (1 - \hat{c}_k^\dagger \hat{c}_k) \hat{c}_k$ using 3rd anticommutator rel.

$= c_k^\dagger \hat{c}_k - \hat{c}_k^\dagger \hat{c}_k^\dagger \hat{c}_k \hat{c}_k$

using 1st anticomm. relation

$= \hat{N}_k^2$ (2)

(g) Operating on a state $|n_1, n_2, \ldots, n_k, \ldots\rangle$ gives

$n_k^2 = n_k \Rightarrow n_k(n_k - 1) = 0 \Rightarrow n_k = 0, 1$ (1) (2)

This is the Pauli exclusion principle.