Advanced Quantum Mechanics

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August 8, 2009

Abstract

These are a set of notes I have made, based on lectures given by S.Grigorenko at the University of Manchester Sept-Dec '08. Please e-mail me with any comments/corrections: jon@jpoffline.com. These notes may be found at www.jpoffline.com.

Contents

1 Opening Remarks

In this course we shall discuss the following:

Different Schemes of QM Here we shall discuss orthodox QM (otherwise known as Copenhagen QM), looking at quantisation & the Schrodinger/Heisenberg pictures of QM. Following that, we shall discuss modern QM (also known as Dirac/Hilbert formalism), via Dirac notation, operator formalism & second quantisation. Finally, we shall look at path integrals.

Symmetries in QM Here, we shall start by looking at transformation operators (translation/rotation), following on to conservation laws and good quantum numbers. And finally, rotation eigenvalues/vectors for orbital and total angular momentum.

Charged Particles & EM Field We look at this by considering a quantum particle in a classical field (the semi-classical approach), via gauge invariance, the Zeeman effect, Landau orbitals, flux quantisation & the Aaromov-Bohm effect. We then look at field quantisation, with the EM field & induced/spontaneous radiation.

2 Weird World of Quantum Mechanics

We shall start by posing the question: "is QM a generalisation of classical physics?". Let us unpack the relevant ideas a little.

2.1 Classical Physics: The Formalism

Classical physics works with material particles, where particles are described by generalised coordinates $q \equiv \{q_i\}$ and momenta $p \equiv \{p_i\}$, where $i = 1, 2, \ldots, n$; the dimension of the system.

The laws of motion in the classical formalism come from two methods: the Lagrangian and Hamiltonian methods. Of course, these methods are not independent.

One obtains the equations of motion in the Lagrangian method by extremising the action

$$S = \int_{t_i}^{t_f} L dt, \qquad L(q, \dot{q}),$$

giving the Euler-Lagrange equations of motion

$$\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = 0.$$

Of course, using our shorthand notation of ignoring the suffix i to denote n equations. In the Hamiltonian method, one extremises the relevant action

$$S = \int p dq - H dt, \qquad H = p\dot{q} - L,$$

where we use the generalised momenta definition

$$p = \frac{\partial L}{\partial \dot{q}}.$$

From the Hamiltonian extremisation method, one finds the Hamiltonian equations of motion

$$\dot{q} = \frac{\partial H}{\partial p}, \qquad \dot{p} = -\frac{\partial H}{\partial q}.$$

In both methods, the underlying principle was the extremisation of the action.

2.2 Classical Physics: The Problems

Now, there are major problems with classical physics, which led to the development of a quantum theory.

Atomic Stability & Atomic Spectra The basic idea behind these problems is pretty simple. Given a proton and electron, they converge on each other, becoming infinitely close together. Hence, given an electron orbiting a nucleus (which has a proton inside), one would assume that the electron will very quickly spiral inwards to join with the proton. This would mean that no atoms are stable. This is quite obviously incorrect. The 'idea' which is wrong in coming to this conclusion, is one regarding the quantisation of electron orbits. Also, a non-quantum model of electron orbits is completely unable to explain the discrete atomic emission spectra observed.

Absence of Magnetism The classical theory is unable to describe the existence of magnetism. A field/force so obviously there in compass needles & bar magnets needs to be explained. The classical theory failed because it was unable to produce the Bohr magneton, which is quantised in units of $\hbar$.

Wrong Black-body Radiation Law Before quantum theory, one only had the Rayleigh-Jeans law of black-body radiation. This law predicted an infinite amount of power to be radiated by photons of increasing frequency. This is also known as the "UV Catastrophe". The solution lies within considering quantum states which photons occupy, and the correct radiation law is the "Planck law".

2.3 Quantum Mechanics: The Formalism

In contrast to classical physics, quantum mechanics works in terms of complex vectors in Hilbert space, $|\psi\rangle$, as opposed to material particles. Such vectors have a complex amplitude of probability of measurement.

The dynamical equation of quantum mechanics is the Schrodinger equation

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

which is linear (the Hamiltonian). The way things are measured is an odd concept: via wavestate collapse. Given some total wavefunction, if we expand it in terms of other states,

$$|\psi\rangle = \sum_n a_n|\psi_n\rangle,$$

then upon measurement, we get result $|\psi_n\rangle$ with probability $|a_n|^2$. This "squared" bit makes quantum measurements non-linear.

From this, we answer our first question: quantum mechanics is not a generalisation of classical physics.

The principle of quantum mechanics is the quantisation procedure.

2.4 Quantum Mechanics: The Paradoxes

There are a few weird predictions of quantum mechanics; we shall briefly outline four of them here.

Wave-particle Duality This is the classic 2-slit experiment. Consider a stream of electrons being fired at a solid barrier with a single slit. On the other side of the barrier is a screen, upon which we observe the electron impacting the screen. From diffraction of the electrons through the slit, there will be an associated probability of finding the electron at a given position on the screen. Now, consider an other slit cut into the barrier, and closing off the first barrier. Now, there will be a different probability of the electron hitting that same position on the screen (it may be further or closer to the barrier). Now, further consider that both slits are open. The probability of the electron hitting the screen at that point is now different to either single-slit case. However, it is neither the straight sum or difference of the individual probabilities. Infact, the probability may disappear altogether. The point is, the electron "is" some wavefunction whose probability distribution means that the probability that it is at some point is not all that intuitive.

Schrodingers Cat Consider a system where there is an atom which randomly makes an electronic transition. During the transition, a photon will be emitted. This photon is then picked up by a photo-multiplier tube, amplified, and a signal sent to a laser, which is aimed at a cat. That is, if the atom transitions, then the laser gets the signal to fire & kill the cat. Further suppose that all this is sealed into a big box, which we cannot open. Now, given that the firing of the laser is governed by a random process, we cannot definitively state wether the state of the cat is "dead" or "alive". Only when we look into the box can we see which state the cat is in. The action of observing the cat "collapses" its wavestate into one of two options (or states). This of course beggars the question of what did the cat look like before we opened the box? This paradox links into the next.

Who Plays God in the Universe? Considering again the dead-alive cat state of before. The actual state was determined by the process of measurement. Without measurement, the cat would have remained in the superposition of the two states. Now, who is the observer in the universe who observes things for which there is noone to observe? That is, who is out there, looking at the random planets/stars/galaxies, collapsing their wavestates into one of the many possible choices? Maybe one concludes that there is noone who does this, leaving the unobserved universe in a perpetual state of "un-collapsed-ness".

The EPR Paradox The acronym stands for "Einstein-Podolsky-Rosen". Consider an atomic transition in which two photons are emitted in opposite directions. The spins of the photons are coupled. That is, if one is "up", the other must be "down", by conservation of

spin. Now, suppose that these photons travel (uninterrupted) for a huge distance. Then, suppose that the spin of one of the photons is measured to be something; then, this measurement collapses the wavestate superposition into one of the observable states. This then immediately forces the other photon into the opposing state. That is, a "singal" is transfered between the photons, instantaneously. This instantaneous signal-sending is an obvious problem in light of Einsteins relativity!

A famous quote by Richard Feynman:
"*It is impossible to understand quantum mechanics, in the end people just get used to it.*"
Notice that this phrase works perfectly well if one substitutes the words "quantum mechanics" for "women".

3 Different Quantisation Schemes

3.1 Orthodox Quantisation

This is also referred to as the Copenhagen interpretation, or conventional quantum mechanics.

The objects are the normalised wavefunction $\psi(x)$, such that

$$\int \psi^*(x)\psi(x)dx = 1,$$

where we still use our multi-dimensional shorthand. Just taking ourselves out of this for a second, then the above will simply read

$$\int \psi^*(x_1, \ldots, x_n)\psi(x_1, \ldots, x_n)dx_1 \ldots dx_n = 1.$$

Where such integrals are understood to be taken over all space.

The dynamic law is the Schrodinger equation,

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \hat{H}\psi(x,t),$$

where the Hamiltonian is the differential operator

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x).$$

The measurement law is such that given eigenfunctions ψ_n of an operator $\hat{Q}$, the probability of a measurement resulting in quantity q_n is given by $|a_n|^2$; upon which the system has collapsed into state ψ_n. The total wavefunction of the system (before measurement) was given by

$$\psi = \sum_i a_n\psi_n.$$

The quantisation principle may be seen as

$$H(p_i, q_i) \longmapsto \hat{H}\left(-i\hbar\frac{\partial}{\partial x_i}, x_i\right).$$

That is, generalised momenta/positions go to the momentum/position operators. This is also known as the correspondence principle.

Problems with this method are four-fold.

- The ordering problem: "usually", $p^2q = ppq = qp^2$. However, the ordering of operators matters (a lot) in quantum mechanics. This is something the above quantisation principle is unable to get right.

- The coordinate choice. Classically, we are at liberty to choose different coordinates; however, such a choice will lead to different operators, and thus different energies.
- Constraint equation. The choice of this is debatable.
- No particle creation/destruction is allowed - which we shall see is a problem.

3.2 Modern Quantum Mechanics

Here, we have objects $|\psi\rangle$ which are state-vectors, dynamics are described by the Schrodinger equation

$$\hat{H}|\psi\rangle = i\hbar\frac{d}{dt}|\psi\rangle,$$

and principle is the quantisation scheme.

We shall now discuss Dirac formalism, with quite a detour into linear algebra.

3.2.1 Dirac Formalism

Taking quite a simple Hamiltonian, the Schrodinger equation is

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla + V(x,t)\right)\psi(x,t) = \hat{H}(x,t)\psi(x,t).$$

Now, writing out what the partial derivative means, in terms of time-steps

$$\psi(x,\Delta t) - \psi(x,0) = -\frac{i}{\hbar}\hat{H}(x,0)\psi(x,0)\Delta t,$$

we see that we can trivially factorise it into

$$\psi(x,\Delta t) = \left(1 - \frac{i}{\hbar}\hat{H}(x,0)\Delta t\right)\psi(x,0).$$

Thus, we see that it is linear. If we consider the next time-step

$$\psi(x,2\Delta t) = \left(1 - \frac{i}{\hbar}\hat{H}(x,\Delta t)\Delta t\right)\psi(x,\Delta t),$$

we see that we can then put in the expression for $\psi(x,\Delta t)$,

$$\psi(x,2\Delta t) = \left(1 - \frac{i}{\hbar}\hat{H}(x,0)\Delta t\right)\left(1 - \frac{i}{\hbar}\hat{H}(x,\Delta t)\Delta t\right)\psi(x,0).$$

This then suggests that we can write the time evolution of the wavefunction as being due to some evolution operator. We denote it as

$$\psi(x,t) = \hat{U}_t\phi(x,0).$$

We can see linearity from this. Consider some initial wavefunction 1, being evolved into its final wavefunction; and consider that this is done to two wavefunctions. That is

$$\psi_{1i} \xrightarrow{\hat{U}_t} \psi_{1f}, \quad \psi_{2i} \xrightarrow{\hat{U}_t} \psi_{2f}.$$

Then, consider a linear combination of the left- and right-hand sides

$$\alpha\psi_{1i} + \beta\psi_{2i} \xrightarrow{\hat{U}_t} \alpha\psi_{1f} + \beta\psi_{2f}.$$

Thus confirming linearity.

Let us consider introducing some basis, $\phi_n(x)$, from which we can develop any function

$$\psi(x,t) = \sum_n a_n(t)\phi_n(x) = \mathbf{a}\cdot\mathbf{e}, \quad \phi_n(x) \equiv e_n.$$

Suppose we evolved the basis e_n, and it ended up giving us some new function

$$\begin{aligned} e_n \xrightarrow{\hat{U}_t} \psi_n(x,t) &= \sum_m U_{nm}(t)\phi_m(x) \\ &= \sum_m U_{nm}(t)e_m. \end{aligned}$$

Further, let us have

$$\psi(x,0) = \sum_n a_n(0)\phi_n(x),$$

and then let us evolve it. That is, the evolution operator acts on the basis, not the coefficient (as it is only at $t = 0$). Thus,

$$\psi(x,0) \xrightarrow{\hat{U}_t} \sum_{n,m} a_n(0)U_{nm}(t)\phi_m(x),$$

which is just $\psi(x,t)$

$$\psi(x,t) = \sum_{n,m} a_n(0)U_{nm}(t)\phi_m(x).$$

Let us denote this back in terms of development into a basis

$$\psi(x,t) = \sum_n a_n(t)\phi_n(x), \quad a_n(t) = \sum_m U_{nm}(t)a_m(0).$$

Therefore, if we know how the basis evolves, we therefore know how any function evolves. This is a direct consequence of linearity.

3.2.2 Vector Spaces

Consider a vector & set of bases

$$\begin{pmatrix} x^1 \\ x^2 \\ x^3 \end{pmatrix}, \quad \{e_i\} = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3).$$

Vectors add, and can be multiplied by a scalar thus

$$\begin{pmatrix} x^1 \\ x^2 \\ x^3 \end{pmatrix} + \begin{pmatrix} y^1 \\ y^2 \\ y^3 \end{pmatrix} = \begin{pmatrix} x^1 + y^1 \\ x^2 + y^2 \\ x^3 + y^3 \end{pmatrix}, \quad \alpha \begin{pmatrix} x^1 \\ x^2 \\ x^3 \end{pmatrix} = \begin{pmatrix} \alpha x^1 \\ \alpha x^2 \\ \alpha x^3 \end{pmatrix}.$$

We can change basis,

$$e \mapsto e' = Ae, \quad \mathbf{e}_i = A^j{}_i \mathbf{e}_j,$$

and similarly coordinates

$$x' = A^{-1}x;$$

where the transformation matrix A satisfies

$$A^{-1}A = 1.$$

We write vectors as a sum over components times basis

$$\mathbf{x} = e \cdot x = \sum_i \mathbf{e}_i x^i.$$

Under change of vector under coordinate & basis transformation, nothing happens

$$\mathbf{x}' = e' \cdot x' = AxA^{-1}e = e \cdot x.$$

The Scalar Product We define the scalar product by giving a rule as to how the basis vectors combine. Thus, for our Cartesian basis

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}.$$

Generally, this is of course just the metric of the basis. Note that this then allows us to write

$$\begin{aligned} \mathbf{x} \cdot \mathbf{y} &= \mathbf{e}_i x^i \cdot \mathbf{e}_j y^j \\ &= x^i y^j \mathbf{e}_i \cdot \mathbf{e}_j \\ &= x^i y^j \delta_{ij} \\ &= x^i y_i. \end{aligned}$$

We write the of a square of a vector as the scalar product of the vector with itself;

$$\mathbf{x} \cdot \mathbf{x} = \sum_i x_i^2.$$

The scalar product is linear in both arguments.

Notice that if $\mathbf{x} = \sum \mathbf{e}_i x^i$, then

$$\begin{aligned} \mathbf{x} \cdot \mathbf{e}_i &= \sum_j x^j \mathbf{e}_j \cdot \mathbf{e}_i \\ &= \sum_j \delta_{ij} x^j \\ &= x_i. \end{aligned}$$

Also,

$$\begin{aligned} \mathbf{x} &= \sum_i \mathbf{e}_i x^i \\ &= \sum_{i,j} \mathbf{e}_i x_j \delta^{ij} \\ &= \sum_{i,j} \mathbf{e}_i (\mathbf{x} \cdot \mathbf{e}_j) \delta^{ij}. \end{aligned}$$

This is merely showing that we can change the basis to make the problem simpler.

Coordinate Transformations Consider that we know x_i in the basis $\mathbf{e}_i$. What are the x'_i in the other basis $\mathbf{e}'_i$?

Now, consider our previous results that $x_i = \mathbf{x} \cdot \mathbf{e}_i$ and that $\mathbf{x} = \mathbf{x}'$. Then, combining the two, we see that

$$x'_i = \mathbf{x} \cdot \mathbf{e}'_i = \sum_j x^j \mathbf{e}_j \cdot \mathbf{e}'_i = \sum_j A_{ij} x^j,$$

where we first just wrote out the vector in terms of its components. We then identified the matrix

$$A_{ij} = \mathbf{e}_i \cdot \mathbf{e}'_j.$$

We can introduce some linear transformation, $y = Tx$; thus

$$y_j = \mathbf{y} \cdot \mathbf{e}_j = T\mathbf{x} \cdot \mathbf{e}_j.$$

Let us now consider complex vector spaces.

3.2.3 Complex Vector Spaces

A complex vector space, with some scalar product rule, such that it gives a complete metric space, is called Hilbert space. We shall do all this under the notation $x = \{x_i\}$.

Scalar Product We define the scalar product thus

$$\int \chi^*(x)\psi(x)dx = \sum_x \chi_x^*\psi_x V_{dx}, \quad V_{dx} = dx = \text{metric}.$$

We have that ψ_x are the components of some vector $|\psi\rangle$, and χ_x^* the components of some complex conjugate (also called the adjoint) vector $\langle\chi|$. Thus, using some sort of abstract vector basis, we have

$$|\psi\rangle = \sum_x \psi_x \mathbf{e}_x, \quad \langle\chi| = \sum_x \chi_x^* \mathbf{e}_x^*.$$

Therefore, notice that

$$\langle\chi|\psi\rangle = \sum_{x,x'} \chi_x^*\psi_{x'}\mathbf{e}_x^* \cdot \mathbf{e}_{x'},$$

and defining that $\mathbf{e}_x^* \cdot \mathbf{e}_{x'} = V_{dx}\delta_{xx'}$, then

$$\langle\chi|\psi\rangle = \sum_x \chi_x^*\psi_x V_{dx} = \int \chi^*(x)\psi(x)dx.$$

Finally, notice that

$$\langle\psi|\chi\rangle = \int \psi^*(x)\chi(x)dx = \left(\langle\chi|\psi\rangle\right)^*.$$

Let us denote the basis $\mathbf{e}_x$ as $|x\rangle$ (such that it only has a unit non-zero entry at the x^{th} element), then

$$\langle x'|x\rangle = \delta_{xx'} = \delta(x' - x);$$

where we shall be flippant with continuous/discrete. This then defines an orthonormal coordinate basis, which we may then develop any function into;

$$|\psi\rangle = \sum_x \psi_x |x\rangle.$$

We use the standard identification that $\psi_x = \psi(x)$. Similarly, we see that

$$\langle\chi| = \sum_x \chi_x^* \langle x|.$$

Restoration of Wavefunction We say that $\langle\chi|$ is adjoint to $|\chi\rangle$. So then, given the components in a basis, what is the wavefunction $\psi(x)$ itself? We proceed thus

$$\begin{aligned}
\langle x|\psi\rangle &= \langle x| \sum_{x'} \psi_{x'}|x'\rangle \\
&= \sum_{x'} \psi_{x'}\langle x|x'\rangle \\
&= \sum_{x'} \psi_{x'}\delta_{xx'} \\
&= \psi_x \equiv \psi(x).
\end{aligned}$$

Therefore, we see that the restoration of the wavefunction is achieved

$$\psi(x) = \langle x|\psi\rangle = \psi_x.$$

Completeness of the Basis Now, consider the development of a state into a basis

$$\begin{aligned} |\psi\rangle &= \sum_x \psi_x |x\rangle \\ &= \sum_x \langle x|\psi\rangle |x\rangle \\ &= \left(\sum_x |x\rangle\langle x|\right)|\psi\rangle, \end{aligned}$$

we thus see that the bracketed quantity must be unity, in order to make the equation consistent. Therefore, we arrive at the completeness of the basis statement

$$\sum_x |x\rangle\langle x| = 1. \tag{3.1}$$

Different Bases Let us introduce some new basis $|n\rangle$, which satisfies orthonormality, $\langle n|m\rangle = \delta_{nm}$. Then, suppose we develop some state in terms of this new basis,

$$|\psi\rangle = \sum_n a_n |n\rangle,$$

then, to find the coefficients a_n, we form the scalar product with "another" element of the basis

$$\langle m|\psi\rangle = \sum_n a_n \langle m|n\rangle = a_m;$$

where we used the above orthonormality relation. Further, consider that

$$\begin{aligned} |\psi\rangle &= \sum_n a_n |n\rangle \\ &= \sum_n \langle n|\psi\rangle |n\rangle \\ &= \left(\sum_n |n\rangle\langle n|\right)|\psi\rangle. \end{aligned}$$

Thus, again, we see the completeness of the basis

$$\sum_n |n\rangle\langle n| = 1.$$

Suppose that we have

$$\langle\chi| = \sum_n b_n \langle n|,$$

then we see that

$$b_n = \langle\chi|n.$$

Similarly, notice that

$$|\psi\rangle = \sum_n a_n |n\rangle \quad \text{conjugate to} \quad \langle\psi| = \sum_n a_n^* \langle n|.$$

Transition Between Bases Now, consider that we have

$$\psi(x,t) = \langle x|\psi\rangle; \quad |\psi\rangle = \sum_n a_n |n\rangle, \quad a_n = \langle n|\psi\rangle;$$

where the first expression is something we want to convert into the basis of the last two. In the final expression, consider inserting something which is unity. Thus consider

$$\begin{aligned} a_n &= \langle n|\psi\rangle \\ &= \langle n| \left(\sum_x |x\rangle\langle x| \right) |\psi\rangle \\ &= \sum_x \langle n|x\rangle \psi(x) \\ &= \sum_x \langle x|n\rangle^* \psi(x) \\ &= \sum_x n^*(x)\psi(x). \end{aligned}$$

The final expression is just the scalar product. And therefore,

$$a_n = \int n^*(x)\psi(x)dx.$$

Discrete .vs. Continuous Suppose that λ is an index describing some basis. It could be continuous or discrete. We use the "generalised Kronecker symbol" when denoting such ambiguities in

$$\langle\lambda|\lambda'\rangle = \delta_{\lambda\lambda'}.$$

The generalised Kronecker symbol is to be used thus:

$$\delta_{\lambda\lambda'} = \begin{cases} \delta_{\lambda\lambda'} & \text{The normal Kronecker delta, if indices discrete,} \\ \delta(\lambda - \lambda') & \text{The Dirac delta, if indices continuous,} \\ 0 & \text{Otherwise.} \end{cases}$$

If $\lambda = \{\lambda_i\}_{i=1}^n$, a multi-index label, then we modify each

$$\delta_{\lambda\lambda'} = \prod_{i=1}^{n} \delta_{\lambda_i\lambda_i'}, \quad \delta(\lambda - \lambda') = \prod_{i=1}^{n} \delta(\lambda_i - \lambda_i').$$

And therefore, giving the required generalised completeness of the basis

$$\sum_{\lambda} |\lambda\rangle\langle\lambda| = 1.$$

Example: Momentum & Position Basis Consider that $|x\rangle$ is the coordinate basis, and that $|p\rangle$ is the momentum basis. Then,

$$\begin{aligned} |\psi\rangle &= \sum_x \psi(x)|x\rangle \\ &= \sum_p \psi(p)|p\rangle. \end{aligned}$$

Then, using the final expression,

$$\begin{aligned} \psi(p) &= \langle p|\psi\rangle \\ &= \sum_x \langle p|x\rangle\langle x|\psi\rangle \\ &= \sum_x \langle p|x\rangle\psi(x). \end{aligned}$$

In the first step, all we did was to insert the usual "unity", and progress that through. Notice then that

$$\langle p|x\rangle = \langle x|p\rangle^* = P^*(x),$$

and that (given $\hat{P}|p\rangle = p|p\rangle$)

$$\langle x|\hat{P}|p\rangle = \langle x|p|p\rangle = p\langle x|p\rangle = pP(x).$$

Let us also insert our "unity" into the first expression,

$$\langle x|\hat{P}|p\rangle = \sum_{x'} \langle x|\hat{P}|x'\rangle\langle x'|p\rangle = -i\hbar \sum_{x'} \frac{d}{dx}\delta_{xx'}P(x') = pP(x).$$

Thus,

$$-i\hbar\frac{dP}{dx} = pP(x),$$

which we fairly easily solve to

$$P(x) = \frac{1}{\left(\sqrt{2\pi\hbar}\right)^n} e^{ipx/\hbar},$$

where n is the dimension of the space in which we are working. Finally, we see that

$$\psi(p) = \sum_x \langle p|x\rangle\psi(x) = \int P^*(x)\psi(x)dx = \frac{1}{\left(\sqrt{2\pi\hbar}\right)^n} \int e^{-ipx/\hbar}\psi(x)dx.$$

3.3 Quantum Mechanical Operators

As we have seen, an operator $\hat{Q}$ is a linear machine which transforms one quantum state into another,

$$\hat{Q} : \psi_i \longmapsto \chi_i.$$

That it is linear implies

$$\hat{Q} : \alpha\psi_1 + \beta\psi_2 \longmapsto \alpha\chi_1 + \beta\chi_2.$$

Now, we have already seen that we can write a quantum state as a development (sum) over an orthonormal basis,

$$|\psi\rangle = \sum_n a_n |n\rangle.$$

Then, then operator acting on the basis

$$\begin{aligned} \hat{Q}|n\rangle &= \sum_m |m\rangle\langle m|\hat{Q}|n\rangle \\ &= \sum_m Q_{mn}|m\rangle, \quad Q_{mn} \equiv \langle m|\hat{Q}|n\rangle. \end{aligned}$$

And thus, the operator acting on a state,

$$\hat{Q}|\psi\rangle = \sum_n a_n \hat{Q}|n\rangle = \sum_{n,m} a_n Q_{mn}|m\rangle.$$

In this way, we say that Q_{mn} is the operator $\hat{Q}$ in $|n\rangle$ representation.

Now, suppose we want to find $\hat{Q}$, if we know Q_{mn}. Then, consider that

$$|\chi\rangle = \hat{Q}|\psi\rangle,$$

inserting two "unities" on the RHS,

$$|\chi\rangle = 1.\hat{Q}.1.|\psi\rangle,$$

that is,

$$|\chi\rangle = \sum_{n,m} |n\rangle\langle n|\hat{Q}|m\rangle\langle m|\psi\rangle.$$

Now, we see Q_{mn} present,

$$\begin{aligned} |\chi\rangle &= \sum_{n,m} |n\rangle Q_{nm}\langle m|\psi\rangle \\ &= \sum_{n,m} Q_{nm}|n\rangle\langle m|\psi\rangle \\ &= \hat{Q}|\psi\rangle. \end{aligned}$$

Thus, it is clear that

$$\hat{Q} = \sum_{n,m} Q_{nm}|n\rangle\langle m|. \tag{3.2}$$

Suppose that Q_{nm} is diagonal (that is, all off-diagonal elements are zero),

$$Q_{nm} = q_n \delta_{nm},$$

then it is clear that

$$\begin{aligned} \hat{Q} &= \sum_{n,m} Q_{nm}|n\rangle\langle m| \\ &= \sum_{n,m} q_n \delta_{nm}|n\rangle\langle m| \\ &= \sum_{n} q_n|n\rangle\langle n|. \end{aligned}$$

Then, we say that $\hat{Q}$ is diagonal in $|n\rangle$ representation;

$$\hat{Q} = \sum_{n} q_n|n\rangle\langle n|. \tag{3.3}$$

3.3.1 Operator Formalism

Here we shall go through more operator formalism & their properties.

The Correspondence Principle For every classical value (i.e. observable), f, there exists a quantum mechanical operator $\hat{f}$. The converse is not true (for example, spin & parity). Thus,

$$f(p,q) \longmapsto \hat{f}\left(-i\hbar\frac{d}{dx}, x\right).$$

The Expected Value An average value of a measured quantity $\hat{Q}$ is given by $\langle\psi|\hat{Q}|\psi\rangle$, given that the system was in the state $|\psi\rangle$ immediately before measurement. Let us show this relation.

Now, we have our state & operator,

$$|\psi\rangle = \sum_{n} a_n|n\rangle, \quad \hat{Q} = \sum q_n|n\rangle\langle n|.$$

Then, with probability $|a_n|^2$, we have outcome q_n. Then, the average value of $\hat{Q}$ (the average denoted with an angled braces), is just the sum over all possible values times the probability of getting that value;

$$\left\langle \hat{Q} \right\rangle = \sum_n q_n |a_n|^2.$$

Now, we have that

$$\langle n|\psi\rangle = \langle n| \sum_n a_n |m\rangle = a_n,$$

so that

$$\begin{aligned} \left\langle \hat{Q} \right\rangle &= \sum_n q_n \left|\langle n|\psi\rangle\right|^2 \\ &= \sum_n q_n \langle n|\psi\rangle \left(\langle n|\psi\rangle\right)^*, \end{aligned}$$

however, $(\langle n|\psi\rangle)^* = \langle\psi|n\rangle$. So,

$$\begin{aligned} \left\langle \hat{Q} \right\rangle &= \sum_n q_n \langle n|\psi\rangle\langle\psi|n\rangle \\ &= \sum_n q_n \langle\psi|n\rangle\langle n|\psi\rangle \\ &= \langle\psi| \left(\sum_n q_n |n\rangle\langle n| \right) |\psi\rangle \\ &= \langle\psi|\hat{Q}|\psi\rangle. \end{aligned}$$

Hence shown.

Hermitian Conjugates For every operator $\hat{Q}$, there exists an Hermitian conjugate $\hat{Q}^\dagger$, which acts to the left. Thus,

$$|\chi\rangle = \hat{Q}|\psi\rangle, \quad \langle\chi| = \langle\psi|\hat{Q}^\dagger.$$

We have used that the Hermitian conjugate of a ket-state is a bra-state.

Now, we have that an operator is

$$\hat{Q} = \sum_{n,m} Q_{nm} |n\rangle\langle m|,$$

then, taking the Hermitian conjugate of the whole expression,

$$\hat{Q}^\dagger = \sum_{n,m} Q^*_{nm} |m\rangle\langle n|.$$

Now then, we have that

$$\langle\chi| = (|\chi\rangle)^\dagger = \left(\hat{Q}|\psi\rangle\right)^\dagger,$$

putting in two unities,

$$\left(\hat{Q}|\psi\rangle\right)^\dagger = \sum_{n,m}\left(|n\rangle\langle n|\hat{Q}|m\rangle\langle m|\psi\rangle\right)^\dagger.$$

Then, we can see that this is

$$\left(\hat{Q}|\psi\rangle\right)^\dagger = \sum_{n,m}\langle n|\hat{Q}|m\rangle^*\langle m|\psi\rangle^*\langle n|,$$

but, $\langle m|\psi\rangle^* = \langle\psi|m\rangle$, so

$$\left(\hat{Q}|\psi\rangle\right)^\dagger = \sum_{n,m}\langle n|\hat{Q}|m\rangle^*\langle\psi|m\rangle\langle n|.$$

Rearranging this,

$$\begin{aligned}\left(\hat{Q}|\psi\rangle\right)^\dagger &= \sum_{n,m}\langle\psi|m\rangle\langle n|\langle n|\hat{Q}|m\rangle^* &(3.4)\\ &= \sum_{n,m}\langle\psi|m\rangle\langle n|Q^*_{nm}. &(3.5)\end{aligned}$$

Now, writing the LHS as

$$\left(\hat{Q}|\psi\rangle\right)^\dagger = \langle\psi|\hat{Q}^\dagger,$$

and expanding out the bra-state in terms of its basis,

$$\langle\psi|\hat{Q}^\dagger = \sum_m a^*_m\langle m|\hat{Q}^\dagger.$$

Then, as $a^*_n = \langle n|\psi\rangle^* = \langle\psi|n\rangle$, we see that this is just

$$\begin{aligned}\langle\psi|\hat{Q}^\dagger &= \sum_m\langle\psi|m\rangle\langle m|\hat{Q}^\dagger\\ &= \sum_{n,m}\langle\psi|m\rangle\langle m|\hat{Q}^\dagger|n\rangle\langle n|\\ &= \sum_{n,m}\langle\psi|m\rangle\langle n|Q^\dagger_{mn}.\end{aligned}$$

So, comparing this with (3.4), we see that

$$(Q^\dagger)_{nm} = Q^*_{mn}. \tag{3.6}$$

Combinations of Operators We state, and the prove, that if

$$\hat{Q} = \hat{A}\hat{B},$$

then

$$\hat{Q}^\dagger = \hat{B}^\dagger \hat{A}^\dagger.$$

So, the proof. Let us have

$$|\chi\rangle = \hat{B}|\psi\rangle,$$

and that

$$|\eta\rangle = \hat{A}|\chi\rangle.$$

Then, it is clear that

$$|\eta\rangle = \hat{A}|\chi\rangle = \hat{A}\hat{B}|\psi\rangle.$$

Now, consider

$$(|\eta\rangle)^\dagger = \left(\hat{A}|\chi\rangle\right)^\dagger,$$

which is just

$$\langle\eta| = \langle\chi|\hat{A}^\dagger.$$

Similarly,

$$\langle\chi| = \langle\psi|\hat{B}^\dagger.$$

And therefore, we see that

$$\langle\eta| = \langle\chi|\hat{A}^\dagger = \langle\psi|\hat{B}^\dagger\hat{A}^\dagger.$$

Therefore, we have proven our assertion. In a similar way, we can prove that

$$\begin{aligned} \hat{Q} = \hat{A}\hat{B}\hat{C} \quad &\Rightarrow \quad \hat{Q}^\dagger = \hat{C}^\dagger\hat{B}^\dagger\hat{A}^\dagger, \\ \hat{Q} = \hat{A}^2\hat{B}^3\hat{C}^{-1/2} \quad &\Rightarrow \quad \hat{Q}^\dagger = (\hat{C}^{-1/2})^\dagger(\hat{B}^\dagger)^3(\hat{A}^\dagger)^2. \end{aligned}$$

Whereby

$$(\langle m|\hat{Q}|n\rangle)^* = \langle n|\hat{Q}^\dagger|m\rangle.$$

Commutators Operators dont generally commute. That is, we cannot change their order.

$$\left[\hat{A}, \hat{B}\right] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}.$$

For example, position & momentum do not commute,

$$[\hat{x}, \hat{p}] = i\hbar.$$

We can also form

$$\left[\hat{A}^2, \hat{B}\right] = \hat{A}\left[\hat{A}, \hat{B}\right] + \left[\hat{A}, \hat{B}\right]\hat{A}.$$

Hermitian Operators An Hermitian operator is one for whom

$$\hat{Q}^\dagger = \hat{Q}, \quad Q^*_{nm} = Q_{mn}.$$

Physical observables correspond to Hermitian operators. This is seen as the eigenvalues of an Hermitian operator are real. Thus, consider

$$q = \langle\psi|\hat{Q}|\psi\rangle; \quad q^* = \langle\psi|\hat{Q}|\psi\rangle^* = \langle\psi|\hat{Q}^\dagger|\psi\rangle = q.$$

Where the last step follows as the Hermitian conjugate of an Hermitian operator is itself. Therefore, $q = q^*$, and therefore, we state

$$q = \langle\psi|\hat{Q}|\psi\rangle \in \mathbb{R}.$$

We shall look more at this in a "few points time".

Unitary Operators Such unitary operators, $\hat{U}$, are such that

$$\hat{U}^\dagger\hat{U} = 1.$$

They are useful, as they conserve the norm. That is, consider

$$|\chi\rangle = \hat{U}|\psi\rangle, \quad \langle\chi| = \langle\psi|\hat{U}^\dagger.$$

Then,

$$\langle\chi|\chi\rangle = \langle\psi|\hat{U}^\dagger\hat{U}|\psi\rangle = 1.\langle\psi|\psi\rangle = 1.$$

Eigenvalues & Eigenstates An eigenvalue equation is such that when an operator operates on an eigenstate, the eigenstate is returned, multiplied by a number;

$$\hat{Q}|\psi\rangle = \lambda|\psi\rangle.$$

Where the eigenstates have a finite norm,

$$\langle\psi|\psi\rangle < \infty.$$

As an example, consider the momentum operator,

$$-i\hbar\frac{d}{dx}\psi = \lambda\psi \quad \Rightarrow \quad \psi = Ce^{i\lambda x/\hbar}.$$

For the exponent to not-diverge, the argument of the exponential must be complex, thus leaving $\lambda \in \mathbb{R}$.

More on Hermitian Operators: Basis Hermitian operators have real eigenvalues; and eigenstates of Hermitian operators form a complete orthonormal basis.

So, we have that

$$\hat{Q} = \sum_n q_n |n\rangle\langle n|.$$

Then, letting $|n\rangle$ be a normalised eigenvector of an Hermitian operator $\hat{Q}$,

$$\hat{Q}|n\rangle = q_n|n\rangle \quad \Rightarrow \quad q_n = \langle n|\hat{Q}|n\rangle.$$

Thus, q_n is the expectation value of $\hat{Q}$, when the system is initially in $|n\rangle$, an eigenstate. Also, the eigenvalue q_n are real (as was previously shown).

Now, to show orthonormality, consider the action of the Hermitian operator on two different eigenstates, each having different eigenvalue (i.e. are non-degenerate);

$$\hat{Q}|n\rangle = q_n|n\rangle, \quad \hat{Q}|m\rangle = q_m|m\rangle.$$

Multiplying the first by $\langle m|$, and the second by $\langle n|$, results in

$$\langle m|\hat{Q}|n\rangle = q_n\langle m|n\rangle, \quad \langle n|\hat{Q}|m\rangle = q_m\langle n|m\rangle.$$

If we take the conjugate of the second expression,

$$(\langle n|\hat{Q}|m\rangle)^* = q_m^*(\langle n|m\rangle)^* \quad \Rightarrow \quad \langle m|\hat{Q}^\dagger|n\rangle = q_m\langle m|n\rangle,$$

noting that the operator is Hermitian, then this is just $\langle m|\hat{Q}|n\rangle = q_m\langle m|n\rangle$. So, subtracting this from the first expression,

$$\langle m|\hat{Q}|n\rangle - \langle m|\hat{Q}|n\rangle = q_n\langle m|n\rangle - q_m\langle m|n\rangle,$$

which is just

$$(q_n - q_m)\langle m|n\rangle = 0.$$

Therefore, given that $q_n \neq q_m$, we see that

$$\langle m|n\rangle = 0.$$

And, if we had chosen suitable normalisation, we can also write

$$\langle n|m\rangle = \delta_{nm}, \quad q_n \neq q_m.$$

Thus, we have completed the proof of the orthonormality of the eigenstates of Hermitian operators. The proof of completeness is hard, and we shall not do it here.

Using orthonormality, we can show that the representation of an Hermitian operator in the basis of its eigenstates, is diagonal. So, writing the operator down, with two unities,

$$\begin{aligned}\hat{Q} &= \sum_{n,m} |n\rangle\langle n|\hat{Q}|m\rangle\langle m| \\ &= \sum_{n,m} |n\rangle\langle n|q_m|m\rangle\langle m| \\ &= \sum_{n,m} q_m|n\rangle\langle n|m\rangle\langle m| \\ &= \sum_{n,m} q_m|n\rangle\delta_{nm}\langle m| \\ &= \sum_{n} q_n|n\rangle\langle n|.\end{aligned}$$

Thus, proven. It is important to note that this was in the basis of eigenstates of the operator, and that the eigenstates were orthonormal.

Finally, suppose that 3 operators commute & are Hermitian. Then, there exists a basis in which all 3 operators are diagonal,

$$\hat{A}|n\rangle = a_n|n\rangle, \quad \hat{B}|n\rangle = b_n|n\rangle, \ldots.$$

3.3.2 The Schrodinger Equation

Let us look at the Schrodinger equation, in light of our previous discussion.

So, we have

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \mathcal{H}(x,t)\psi(x,t),$$

the RHS of which we write as

$$\mathcal{H}(x,t)\psi(x,t) = \sum_{x'} \mathcal{H}_{xx'}\delta_{xx'}\psi(x',t).$$

In writing this, we are taking the usual Hamiltonian (kinetic plus potential), and writing as a sum. We are not forcing it to be diagonal, as it isnt (for example, in spherical polars).

We write

$$\mathcal{H}_{xx'}\delta_{xx'} = \langle x|\hat{\mathcal{H}}|x'\rangle.$$

Then, putting this in, and multiplying by a bra state,

$$i\hbar\frac{\partial}{\partial t}\langle x|\psi\rangle = \sum_{x'}\langle x|\hat{\mathcal{H}}|x'\rangle\langle x'|\psi\rangle.$$

Now, we notice that (a) we can cancel the $\langle x|$, and that (b) we see unity in $|x'\rangle\langle x'|$. So, the above becomes

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{\mathcal{H}}|\psi\rangle. \tag{3.7}$$

Thus, the Schrodinger equation. We also denote it

$$i\hbar|\dot{\psi}\rangle = \hat{\mathcal{H}}|\psi\rangle.$$

Now, we have that

$$\langle x|\psi\rangle = \psi(x,t), \quad \mathcal{H}_{xx'}\delta_{xx'} = \langle x|\hat{\mathcal{H}}|x'\rangle.$$

Then, putting two unities either side of the Hamiltonian,

$$\hat{\mathcal{H}} = \sum_{x,x'} |x\rangle\langle x|\hat{\mathcal{H}}|x'\rangle\langle x'|,$$

which is clearly,

$$\begin{aligned}\sum_{xx'} |x\rangle\langle x|\hat{\mathcal{H}}|x'\rangle\langle x'| &= \sum_{x,x'} |x\rangle\mathcal{H}_{xx'}\delta_{xx'}\langle x'| \\ &= \sum_{x,x'} \mathcal{H}_{xx'}\delta_{xx'}|x\rangle\langle x'| \\ &= \sum_{x,x'} \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\delta_{xx'}|x\rangle\langle x'|.\end{aligned}$$

3.3.3 Properties of the Hamiltonian

The Hamiltonian is an Hermitian operator,

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}^\dagger,$$

which is clear as it corresponds to energy. The corresponding eigenvalue equation is

$$\hat{\mathcal{H}}|\psi\rangle = E|\psi\rangle, \quad E \in \mathbb{R}.$$

Where E is the energy of the system.

Let $|n\rangle$ be an orthonormal basis of energy eigenstates

$$\hat{\mathcal{H}}|n\rangle = E_n|n\rangle.$$

Then,

$$|\psi\rangle = e^{-iE_nt/\hbar}|n\rangle$$

satisfies the Schrodinger equation. So, the Schrodinger equation is

$$i\hbar|\dot{\psi}\rangle = E_n|\psi\rangle,$$

and thus

$$\hat{\mathcal{H}}|\psi\rangle = E_n|\psi\rangle.$$

To see this, consider that

$$|\psi\rangle = e^{-iE_nt/\hbar}|n\rangle \quad \Rightarrow \quad |\dot{\psi}\rangle = -\frac{iE_n}{\hbar}|\psi\rangle,$$

the RHS expression obviously rearranges into

$$i\hbar|\dot{\psi}\rangle = E_n|\psi\rangle.$$

Now,

$$|\psi\rangle = \sum_n a_n e^{-iE_nt/\hbar}|n\rangle$$

is also a solution to the Schrodinger equation.

Now, notice that

$$|\psi(t=0)\rangle = \sum_n a_n|n\rangle \quad \Rightarrow \quad a_n = \langle n|\psi(0)\rangle,$$

and therefore that

$$|\psi\rangle = \sum_n \langle n|\psi(0)\rangle e^{-iE_nt/\hbar}|n\rangle$$

is also a solution, for all initial states. Rearranging this slightly,

$$|\psi\rangle = \sum_n e^{-iE_nt/\hbar}|n\rangle\langle n|\psi(0)\rangle = \hat{U}(t)|\psi(0)\rangle, \tag{3.8}$$

where we have defined the (unitary; but more on this later) evolution operator

$$\hat{U}(t) \equiv \sum_n e^{-iE_nt/\hbar}|n\rangle\langle n|. \tag{3.9}$$

Note, we can write the Hamiltonian as

$$\hat{\mathcal{H}} = \sum_n E_n|n\rangle\langle n|.$$

3.4 Quantum Evolution

3.4.1 The Schrodinger Picture

Let us start by stating the Schrodinger equation & the result derived above,

$$i\hbar|\dot{\psi}\rangle = \hat{\mathcal{H}}\psi, \quad |\psi\rangle = \hat{U}(t)|\psi(0)\rangle.$$

Now, the Schrodinger equation may be "solved"

$$i\hbar\dot{x} = \hat{\mathcal{H}}x \quad \Rightarrow \quad x = e^{-\frac{i}{\hbar}\int\hat{\mathcal{H}}dt}x(0).$$

So that by the correspondence principle,

$$|\psi\rangle = e^{-\frac{i}{\hbar}\int\hat{\mathcal{H}}dt}|\psi(0)\rangle.$$

Now, if the Hamiltonian is not a function of time, then this is just

$$|\psi\rangle = e^{-\frac{it}{\hbar}\hat{\mathcal{H}}}|\psi(0)\rangle.$$

So, we see that the evolution operator is

$$\hat{U} = e^{-\frac{it}{\hbar}\hat{\mathcal{H}}}, \quad \hat{U}^\dagger = e^{\frac{it}{\hbar}\hat{\mathcal{H}}}.$$

Notice that this operator is unitary, as

$$\hat{U}^\dagger\hat{U} = 1.$$

Thus, notice that

$$\langle\psi|\psi\rangle = \langle\psi(0)|\hat{U}^\dagger\hat{U}|\psi(0)\rangle = 1.$$

So, the Schrodinger picture of quantum mechanics is just this. The state of the system evolves, with the Hamitonian (or, any operator) being constant in time.

3.4.2 The Heisenberg Picture

Here, consider

$$q(t) = \langle\psi(t)|\hat{Q}|\psi(t)\rangle,$$

and that the states are found via the evolution operator,

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle,$$

so that

$$q(t) = \langle\psi(0)|\hat{U}^\dagger(t)\hat{Q}\hat{U}(t)|\psi(0)\rangle.$$

Then, if we define some new operator, which is a function of time

$$\hat{Q}(t) \equiv \hat{U}^{\dagger}(t)\hat{Q}\hat{U}(t),$$

then we have

$$q(t) = \langle\psi(0)|\hat{Q}(t)|\psi(0)\rangle.$$

So now, we have that the operator evolves in time, rather than the state.

So, we have the Heisenberg equation,

$$\frac{d}{dt}\hat{Q}(t) = \frac{\partial\hat{Q}}{\partial t} - \frac{i}{\hbar}\left[\hat{Q}, \hat{\mathcal{H}}\right]. \tag{3.10}$$

Sometimes the time dependent Heisenberg operator is denoted $\hat{Q}_{\hat{\mathcal{H}}}(t)$, to distinguish it from the static $\hat{Q}$.

3.4.3 The Dirac Picture

This picture is also called the interaction picture.

Here, we consider the Hamiltonian to be a sum of a known Hamiltonian, and an interaction potential,

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{V}(t).$$

So, we have our evolution operator, $\hat{U}_0$, due to the known Hamiltonian $\hat{\mathcal{H}}_0$,

$$\hat{U}_0(t) = e^{-\frac{i}{\hbar}\hat{\mathcal{H}}_0 t}.$$

Then, taking our expectation value, and inserting two unities,

$$q(t) = \langle\psi(t)|\hat{U}_0\hat{U}_0^{\dagger}\hat{Q}\hat{U}_0\hat{U}_0^{\dagger}|\psi(t)\rangle,$$

defining a new state vector,

$$|\tilde{\psi}(t)\rangle \equiv \hat{U}_0^{\dagger}|\psi(t)\rangle,$$

and operator,

$$\tilde{\hat{Q}} \equiv \hat{U}_0^{\dagger}\hat{Q}\hat{U}_0,$$

then it is clear that

$$q(t) = \langle\tilde{\psi}(t)|\tilde{\hat{Q}}|\tilde{\psi}(t)\rangle.$$

Then, the Schrodinger equation, in the interaction picture, is

$$i\hbar\frac{d}{dt}|\tilde{\psi}(t)\rangle = \tilde{\hat{V}}|\tilde{\psi}(t)\rangle.$$

So, we have evolution due to the interaction operator.

3.4.4 Examples

Here we shall consider various examples for changing basis for operators.

Momentum in Momentum-representation The general form for the momentum operator is

$$\hat{p} = -i\hbar \sum_{x,x'} \frac{d}{dx} \delta_{xx'} |x\rangle\langle x'|,$$

and

$$p_{xx'} = -i\hbar \frac{d}{dx'} \delta_{xx'}.$$

Now, the momentum operator acting on a state gives a new state,

$$\hat{p}|\psi\rangle = |\chi\rangle.$$

Projecting this into x-representation,

$$\langle x|\hat{p}|\psi\rangle = \langle x|\chi\rangle \equiv \chi(x).$$

Now, let us insert a unity on the LHS,

$$\sum_{x'} \langle x|\hat{p}|x'\rangle\langle x'|\psi\rangle.$$

Now, this is just

$$\sum_{x'} p_{xx'}\psi(x') = -i\hbar \sum_{x'} \frac{d}{dx'} \delta_{xx'}\psi(x'),$$

which is clearly just

$$-i\hbar \frac{d}{dx}\psi(x).$$

And this is the result of acting the momentum operator on $\psi(x)$, in x-representation.

Let us consider for p-representation. So,

$$\hat{p} = \sum_{p,p'} |p\rangle\langle p|\hat{p}|p'\rangle\langle p'|,$$

after inserting two unities. Now, we have the eigenvalue equation, in p-representation,

$$\hat{p}|p\rangle = p|p\rangle.$$

Therefore, we see that the term $\hat{p}|p'\rangle = p'|p'\rangle$, and thus that

$$\hat{p} = \sum_{p,p'} p'|p\rangle\langle p|p'\rangle\langle p'|.$$

However, we are working an orthonormal basis, so

$$\hat{p} = \sum_{p,p'} p'|p\rangle\delta_{pp'}\langle p'| = \sum_{p} p|p\rangle\langle p|.$$

Thus, the momentum operator, in p-representation, is diagonal, as expected.

Now, the wavefunction in p-representation is

$$\langle p|\psi\rangle = \psi(p) \equiv a(p).$$

This is continuous, as momentum is continuous. Notice that in n-representation (for energy),

$$\langle n|\psi\rangle = a_n.$$

Now, consider acting $\hat{p}$ onto $a(p)$, in p-representation. Then,

$$\hat{p}a(p) = \sum_{p'} p\delta_{pp'}a(p) = pa(p),$$

as $\hat{p}$ is diagonal in p-representation. Therefore, it is easy to see that

$$\hat{p}^2a(p) = p^2a(p).$$

Kinetic Energy in p-representation Consider the kinetic energy operator,

$$\frac{\hat{p}^2}{2m},$$

in p-representation. So,

$$\hat{p}^2 = \sum_{p} p^2|p\rangle\langle p|,$$

Then,

$$\frac{\hat{p}^2}{2m}a(p) = \frac{p^2}{2m}a(p).$$

Hence, the kinetic energy in momentum-space is pretty simple.

Interaction $\hat{V}(x)$ in p-representation Now, consider

$$\hat{V}(x) = \sum_{p,p'} |p\rangle\langle p|\hat{V}(x)|p'\rangle\langle p'|,$$

putting in another two unities,

$$\hat{V}(x) = \sum_{p,p',x,x'} |p\rangle\langle p|x\rangle\langle x|\hat{V}(x)|x'\rangle\langle x'|p'\rangle\langle p'|.$$

Now, notice the terms

$$\langle x|\hat{V}(x)|x'\rangle = V(x)\langle x|x'\rangle = V(x)\delta_{xx'}, \quad \langle x|p\rangle = p(x) = C.e^{ipx/\hbar}$$

Thus,

$$\hat{V}(x) = \sum_{p,p',x} |p\rangle C^* e^{-ipx/\hbar} V(x) C e^{ip'x/\hbar} \langle p'|,$$

which is just

$$\hat{V}(x) = |C|^2 \sum_{p,p',x} e^{-\frac{i}{\hbar}x(p-p')} V(x)|p\rangle\langle p'|.$$

Now, we shall send the sum on x to an integral on x,

$$\hat{V}(x) = |C|^2 \sum_{p,p'} \int e^{-\frac{i}{\hbar}x(p-p')} V(x)dx|p\rangle\langle p'|.$$

Let us now define the integral to be

$$V_{p-p'} \equiv |C|^2 \int e^{-\frac{i}{\hbar}x(p-p')} V(x)dx,$$

which is just the Fourier transform of the potential. Thus,

$$\hat{V}(x) = \sum_{p,p'} V_{p-p'}|p\rangle\langle p'|.$$

Notice that it is not diagonal. We denote $q \equiv p - p'$, so that

$$V_q \equiv |C|^2 \int e^{-\frac{i}{\hbar}xq} V(x)dx, \tag{3.11}$$

We can display this pictorially. We denote a bra-state as a line pointing towards the right, with a vertex at the right; a ket-state as a line pointing towards the right, vertex on the left; and a wavey line pointing downwards to its vertex, as V_q, where $q = p - p'$. See the figure.

So, we have

$$\chi(p) = \sum_{p'} V_{p-p'} a(p').$$

As a simple example, consider the potential

$$V(x) = -u_0\delta(x).$$

Then,

$$V_q = -|C|^2 \int e^{-\frac{i}{\hbar}xq} u_0\delta(x)dx = -|C|^2 u_0.$$

The Dirac-delta forces x to be zero.

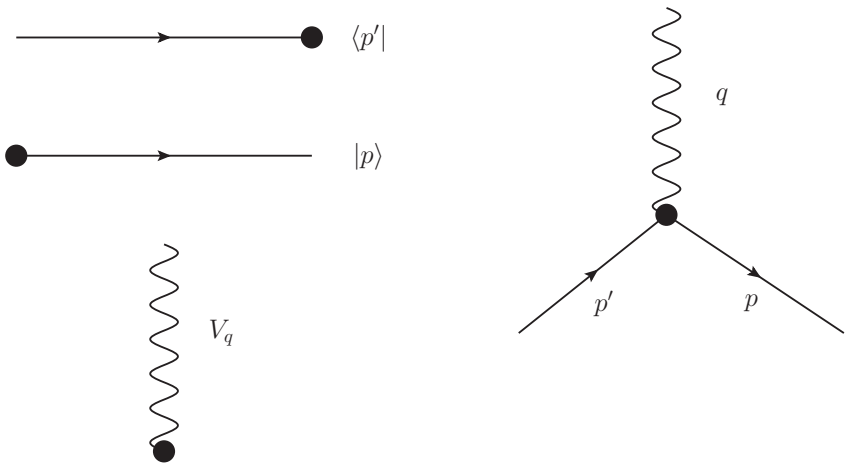

Figure 3.1: Representation of the interaction picture. Notice that at the vertex momentum is conserved.

A Simple Hamiltonian Consider the Hamiltonian, having deep potential spike,

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} - u_0\delta(x),$$

then, in p-representation, it is

$$\hat{\mathcal{H}} = \sum_{p,p'} \frac{p^2}{2m}|p\rangle\langle p'|\delta_{pp'} - \sum_{p,p'} cu_0|p\rangle\langle p'|.$$

Under trivial rearrangement,

$$\hat{\mathcal{H}} = \sum_{p,p'} \left(\frac{p^2}{2m}\delta_{pp'} - cu_0\right)|p\rangle\langle p'|.$$

Now, for eigenvalues, the Hamiltonian has

$$\hat{\mathcal{H}}|\psi\rangle = E|\psi\rangle,$$

projecting onto p-representation,

$$\langle p|\hat{\mathcal{H}}|\psi\rangle = E\langle p|\psi\rangle = Ea(p).$$

Therefore, using our Hamiltonian, the LHS easily becomes

$$\langle p|\sum_{p'',p'} \left(\frac{p''^2}{2m}\delta_{p''p'} - cu_0\right)|p''\rangle\langle p'|\psi\rangle = Ea(p).$$

We thus see that (also noting $\langle p'|\psi\rangle = a(p')$),

$$\begin{aligned}
&\langle p|\sum_{p'',p'}\frac{p''^2}{2m}\delta_{p'p''}|p''\rangle a(p') - \langle p|\sum_{p'',p'}cu_0|p''\rangle a(p') = Ea(p),\\
\Rightarrow &\sum_{p'',p'}\frac{p''^2}{2m}\delta_{p'p''}\langle p|p''\rangle a(p') - \sum_{p'',p'}cu_0\langle p|p''\rangle a(p') = Ea(p),\\
\Rightarrow &\sum_{p'',p'}\frac{p''^2}{2m}\delta_{p'p''}\delta_{pp''}a(p') - \sum_{p'',p'}cu_0\delta_{pp''}a(p') = Ea(p).
\end{aligned}$$

Thus,

$$\frac{p^2}{2m}a(p) - cu_0\sum_{p'}a(p') = Ea(p).$$

Now, we turn the sum over p' into an integral,

$$\frac{p^2}{2m}a(p) - cu_0\int a(p')dp' = Ea(p),$$

rearranging,

$$a(p) = -\frac{cu_0}{E - \frac{p^2}{2m}}\int a(p')dp',$$

integrating,

$$\int a(p)dp = -\int\frac{cu_0}{E-\frac{p^2}{2m}}dp\int a(p')dp'.$$

Now, if we change symbol on the LHS, putting primes on everything, we get

$$\int a(p')dp' = -\int\frac{cu_0}{E-\frac{p^2}{2m}}dp\int a(p')dp',$$

which immediately implies that

$$-\int\frac{cu_0}{E-\frac{p^2}{2m}}dp = 1,$$

absorbing the minus sign, with a modulus on the energy,

$$\int\frac{cu_0}{|E|+\frac{p^2}{2m}}dp = 1.$$

Therefore, we effectively have a condition for what energy levels exist in a system. Note that we have not specified anywhere the dimension of the system, thus, this holds in any dimension of p.

So, in 1D, we have simply,

$$cu_0 \int \frac{dp}{|E| + \frac{p^2}{2m}} = \frac{2\pi c u_0 2m}{2\sqrt{2m|E|}} = 1,$$

which is

$$|E| = 2mc^2 u_0 \pi^2.$$

In 2D we have that $dp = 2\pi p dp$, so that

$$cu_0 \int \frac{2\pi p dp}{|E| + \frac{p^2}{2m}} = cu_0 2\pi \ln |E| = 1,$$

thus,

$$E = e^{-1/2\pi c u_0}.$$

Finally, in 3D, $dp = 4\pi p^2 dp$, does not have a solution. There are no energy levels in 3D.

The power of this method seems obvious now. We do a small amount of algebra, and the result is applicable for many dimensions.

Position-momentum Commutators Let $\hat{x}$ be the position operator in the Schrodinger picture. We want to know $\hat{x}(t)$ (i.e. in the Heisenberg picture). We assume free particles, so that the Hamiltonian reads

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m}.$$

Now, we have that

$$\frac{d\hat{x}}{dt} = \frac{\partial \hat{x}}{\partial t} - \frac{i}{\hbar}\left[\hat{x}, \hat{\mathcal{H}}\right].$$

Now, the important commutator here is

$$\left[\hat{x}, \hat{p}^2\right] = -\hat{p}\left[\hat{p}, \hat{x}\right] - \left[\hat{p}, \hat{x}\right]\hat{p} = 2i\hbar\hat{p}$$

Therefore,

$$\frac{d\hat{x}}{dt} = -\frac{i}{\hbar}\frac{2i\hbar}{2m}\hat{p} = \frac{\hat{p}}{m}.$$

Notice that this is just the classical expression for momentum,

$$m\dot{\hat{x}} = \hat{p}.$$

In a similar way, we can derive that

$$\frac{d\hat{p}}{dt} = \dot{\hat{p}} = 0.$$

Thus, we see conservation of momentum. So, momentum is a constant $\hat{p}_0$. Hence, as

$$\dot{\hat{x}} = \frac{\hat{p}_0}{m} \quad \Rightarrow \quad \hat{x} = \hat{x}_0 + \frac{\hat{p}_0 t}{m}.$$

3.5 Path Integrals

In previous formulations of quantum mechanics, constraints on the system are hard to deal with. So, we develop a new formalism, which is independent of the Hamiltonian, where it is now easy to incorporate constraints.

So, we have that

$$|\psi(t')\rangle = \hat{U}(t',t)|\psi(t)\rangle.$$

Projecting into x-representation,

$$\langle x'|\psi(t')\rangle = \langle x'|\hat{U}(t',t)|\psi(t)\rangle,$$

inserting a unity,

$$\begin{aligned}\psi(x',t') &= \sum_x \langle x'|\hat{U}(t',t)|x\rangle\langle x|\psi(t)\rangle \\ &= \sum_x \langle x'|\hat{U}(t',t)|x\rangle\psi(x,t).\end{aligned}$$

Now, if we send the sum on x to an integral,

$$\psi(x',t') = \int \langle x'|\hat{U}(t',t)|x\rangle\psi(x,t)dx.$$

Now, let us define a *propagator*,

$$K(x',t';x,t) \equiv \langle x'|\hat{U}(t',t)|x\rangle, \tag{3.12}$$

then we have

$$\psi(x',t') = \int K(x',t';x,t)\psi(x,t)dx.$$

Those familiar with Green functions will notice that the propagator is a Green function. The propagator is an evolution operator, in x-representation. So, by our definition of the evolution operator,

$$\hat{U}(t',t) = e^{-\frac{i}{\hbar}\hat{\mathcal{H}}(t'-t)},$$

the propagator is just

$$\begin{aligned}K(x',t';x,t) &= \langle x'|e^{-\frac{i}{\hbar}\hat{\mathcal{H}}t'}e^{\frac{i}{\hbar}\hat{\mathcal{H}}t}|x\rangle \\ &= \langle x'|e^{-\frac{i}{\hbar}\hat{\mathcal{H}}t'}|x,t\rangle \\ &= \langle x',t'|x,t\rangle.\end{aligned}$$

That is, we introduce a time dependent basis. So,

$$K(x',t';x,t) = \langle x',t'|x,t\rangle. \tag{3.13}$$

The basis is normal, as

$$\sum_x |x,t\rangle\langle x,t| = 1.$$

We can see this another way. Consider that

$$\psi(x',t') = \langle x',t'|\psi\rangle,$$

and inserting a unity,

$$\psi(x',t') = \sum_x \langle x',t'|x,t\rangle\langle x,t|\psi\rangle,$$

which is just our definition of the propagator,

$$\psi(x',t') = \sum_x K(x',t';x,t)\psi(x,t);$$

having also noticed that $\langle x,t|\psi\rangle = \psi(x,t)$.

Now, we can derive an interesting relation. Consider the definition of the propagator, (3.13), inserting a unity,

$$K(x',t';x,t) = \langle x',t'|x,t\rangle = \sum_{x''} \langle x',t'|x'',t''\rangle\langle x'',t''|x,t\rangle,$$

however, we see another propgator,

$$K(x',t';x,t) = \sum_{x''} K(x',t';x'',t'')K(x'',t'';x,t).$$

Sending the sum to an integral,

$$K(x',t';x,t) = \int K(x',t';x'',t'')K(x'',t'';x,t)dx''.$$

Let us change notation slightly. We can see that the propagator on the LHS goes from unprimed to single primed, and that in the integrand there is a propagator which goes to some intermediate state (the double primes). So, let us denote the above equation as

$$K(F;I) = \int K(F;1)K(1;I)dx_1.$$

This is the *Markovian property*. Those familiar with advanced statistical mechanics will recognise this property.

The integral sweeps over all possible intermediate states, in order that a transition from one state to the next is made. Infact, we can insert another two unities,

$$\langle F|I\rangle = \sum_{1,2} \langle F|2\rangle\langle 2|1\rangle\langle 1|I\rangle,$$

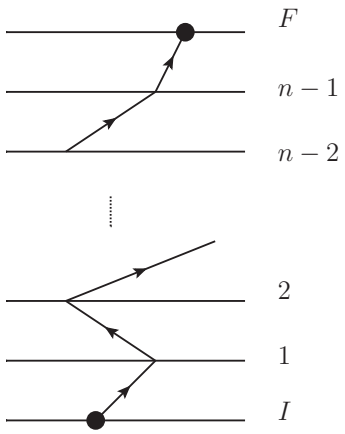

Figure 3.2: Representation of the path integral formulation. The integrals sweep over all possible ways of making each transition. That is, the line joining I and1 sweeps over all possible states in 1; and continuing up to the final state.

so that the corresponding integral will sweep over another combination of intermediate states. We keep inserting unities,

$$K(F;I) = \int K(F;n-1)K(n-1;n-2)\ldots K(1;I)dx_1\ldots dx_{n-1}.$$

So, we connect two points by integrating over all possible trajectories, all possible ways, of getting there. Infact, we also sum over all intermediate states as well.

For a small time interval, the individual amplitude is

$$K(m+1;m) = \frac{1}{(2\pi\hbar)^n}\int dp e^{\frac{i}{\hbar}Ldt},$$

where L is the classical Lagrangian, and n the dimension of the system. Thus, putting all these little pieces together,

$$K(F;I) = \lim_{N\to\infty}\int dx_1\ldots dx_{N-1}\prod_j\int\frac{dp_j}{(2\pi\hbar)^n}e^{\frac{i}{\hbar}\int Ldt},$$

which we denote as

$$K(F;I) = \int\frac{\mathcal{D}x\mathcal{D}p}{(2\pi\hbar)^n}e^{\frac{i}{\hbar}S},$$

where S is the action. We can write this as

$$K(F;I) = \sum_{x_i,p_i} e^{\frac{i}{\hbar}S}.$$

Now, if we have that

$$p_i = m\frac{x_{i+1}-x_i}{t_{i+1}-t_i},$$

then the action is

$$S = \int pdx - \mathcal{H}dt = \sum_i p(x_{i+1} - x_i) - \mathcal{H}(t_{i+1} - t_i),$$

where we have just used the sum-integral cross-over idea.

The advantages of this quantisation scheme, are that there are no problems when introducing constraints. Also, the transition between classical physics & quantum physics is transparent. However, a disadvantage is that the method is mathematically vulnerable (read: works, but shouldn't). The mathematics was developed by physicists, for physics (rather than by mathematicians, then adapted for physics). As a result, the maths wasn't well defined at all, with huge ambiguity, with no-one really understanding why the maths worked at all. It has, however, been mathematically understood a little more.

3.5.1 Classical or Quantum Action?

Now, consider some path, defined by $(x_1(t), p_1(t))$. The associated action is just $S_i(x_1(t), p_1(t))$. The contribution to the path integral will be $e^{\frac{i}{\hbar}S_1}$. Now, consider another path,

$$x_2(t) = x_1(t) + \delta x_1(t), \quad p_2(t) = p_1(t) + \delta p_1(t);$$

where it is clear that the new path is very close to the old one. Then, its contribution will be

$$e^{\frac{i}{\hbar}S_2} = \cos\frac{S_2}{\hbar} + i\sin\frac{S_2}{\hbar}.$$

Then, one will see that such a "total path integral" will have terms such as

$$\frac{\delta S}{\hbar} = \frac{S_1 - S_2}{\hbar}.$$

This is just an oscillatory term (also, the expectation values of cos & sin are both zero). Hence, $\delta S = 0$. Therefore, these trajectories contribute most to the integral. That is, the path for whom the variation in the action is zero, is just given by the Euler-Lagrange equations. This is the classical trajectory.

So, if we let $\frac{S}{\hbar} \gg 1$, then $e^{\frac{i}{\hbar}S_{cl}}$ is the main contributor to the path integral. This is because the oscillatory argument holds. Note that if $\frac{S}{\hbar} \ll 1$, then the oscillatory argument breaks down, and we have deviation from the classical path.

Therefore, we see that (by our rather wooly-argument), the realm of classical physics is $S \gg \hbar$, and of quantum physics for when $S \ll \hbar$.

So, the "semi-classical" value of the propagator is

$$K(F; I) = Ce^{\frac{i}{\hbar}S_{cl}},$$

where C is a constant, and S_{cl} the classical action. That is, the above statement says that the only path to contribute is the classical one. Consider the standard spring Lagrangian; upon solving, one finds an equation of motion. This is the classical path. Our statement above states that the classical path is the main contributor for systems where the action is a lot greater than $\hbar$. However, if this were not the case, the spring would also have motion not described by the standard oscillatory expression.

The classical action, for a free particle, reads

$$S_{cl} = px - \mathcal{H}t \quad \Rightarrow \quad \frac{S_{cl}}{\hbar} = x\frac{p}{\hbar} - \frac{\mathcal{H}}{\hbar}t.$$

Now, using the standard expressions, $E = \hbar\omega$ (noting that the Hamiltonian is the energy), and $p = \hbar k$, we see that

$$\frac{S_{cl}}{\hbar} = kx - \omega t.$$

Therefore, the corresponding propagator is just

$$K(F;I) = Ce^{\frac{i}{\hbar}S_{cl}} = Ce^{-i(\omega t - kx)},$$

that is, a plane wave.

A Free Particle Consider a free particle, which travels from the initial state, I, to final state F; where each has position & time $I(x_i, t_i), F(x_f, t_f)$. Suppose that the total length of the path is L, and time T. Then, the speed of the particle is just

$$v = \frac{L}{T} = \frac{x_f - x_i}{t_f - t_i}.$$

Now, the classical momentum is just

$$p_{cl} = mv = \frac{mL}{T}.$$

So, the classical action is

$$S_{cl} = \int_i^f pdx - \mathcal{H}dt,$$

if we use the standard $v = dx/dt$, then this is just

$$S_{cl} = \int_i^f (pv - \mathcal{H})dt.$$

Now, we use that

$$v = \frac{p}{m}, \quad \mathcal{H} = \frac{p^2}{2m},$$

then we see that

$$S_{cl} = \int_i^f \left(\frac{p^2}{m} - \frac{p^2}{2m} \right) dt,$$

which evaluates easily to

$$S_{cl} = \frac{p^2}{2m} T,$$

after noting that momentum p is constant. So, if we insert our expression for p, the classical action is

$$S_{cl} = \frac{mL^2}{2T}.$$

Then, if $S_{cl} \gg \hbar$, the only contributor to the propagator is the classical action;

$$K(F;I) = Ce^{i\frac{mL^2}{2T\hbar}}, \quad S_{cl} \gg \hbar.$$

Using our previous definitions of the length & time of the path, this is obviously just

$$K(F;I) = Ce^{i\frac{m(x_f - x_i)^2}{2(t_f - t_i)\hbar}}.$$

So, let is consider two examples, to test if they are quantum or classical in nature.

- An electron in a scanning electron microscope. Here, typical energies are $E \approx 3$keV, length scale $L \approx 50$cm. If we use that $E = \frac{1}{2}mv^2$, $T = L/v$, $E = \frac{p^2}{2m} = \frac{1}{2}mv^2$, then we can find that $\frac{S_{cl}}{\hbar} \approx 10^{10}$. Therefore, such a system is (very!) classical.
- An electron in a quantum well. Here, considering that typical energies are 3meV, length scales 1nm, we find that $\frac{S}{\hbar} \approx 0.6$. Therefore, such a system is quantum in nature.

Parabolic Potential & Tunelling Let us first consider a parabolic potential (quantum harmonic oscillator), and determine how energy levels arise.

Now, if we consider that

$$\sum_n e^{i\frac{S}{\hbar}n} = 0,$$

unless $\frac{S}{\hbar}$ is an integer multiple of 2π; then, it is easy to see that the levels will be quantised.

Now, consider a particle tunneling between two wells (looks like a mexican hat potential). Then, the energy levels in one well are just $S_{cl} = 2\pi m\hbar$.
Now, if the action is complex, then the propagator decays. This case arises when we consider that between the wells (at the "hump"), a particle will have complex momentum (in order to keep the energy - sum over potential & kinetic - zero). Then, there are infact "degenerate trajectories". That is, ones for whom at different times, the position is the same. It is because it gets infinitely "hard" to get to the "hump". A degenerate trajectory is such that

$$x(t) \approx x(t + \tau).$$

So, the total propagator is formed from two terms. One for motion within wells, and one between wells. This looks like

$$K(F;I) = e^{i\frac{S}{\hbar}} + \tau e^{-\frac{S}{\hbar}},$$

respectively. The "i" is missing from the second term as the action is complex between the wells.

3.6 Review of Quantisation Schemes

Let us review the quantisation schemes we have discussed.

Copenhagen Interpretation The main equation was the Schrodinger equation, in the form

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi = i\hbar\dot{\psi},$$

where the advantages of the quantisation scheme are that of being very well developed. It has applications in 1D & 2D, but 3D problems tend to be hard to solve. Disadvantages of the scheme are in measurement & quantisation.

Dirac Formalism The main equation here, is the Schrodinger equation in the form

$$i\hbar|\dot{\psi}\rangle = \hat{\mathcal{H}}|\psi\rangle.$$

This formalism is mathematically sound, and has applications in many body-problems. However, the disadvantages are the same as the Copenhagen interpretation: within measurement & quantisation. It is also difficult to incorporate equations of constraint.

Path Integrals Here, the main equation is that for the propagator

$$K(F;I) = \int \frac{\mathcal{D}x\mathcal{D}p}{(2\pi\hbar)^n} e^{\frac{i}{\hbar}S}.$$

The advantage of this scheme is that it is physically very transparent. However, problems come in mathematical rigour. The formalism has applications within elementary particles & fields.

4 Quantum Harmonic Oscillator

We shall look at the harmonic oscillator, and find its eigenstates & eigenvalues, using raising & lowering operators.

The classical Hamiltonian for a harmonic oscillator is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2,$$

therefore, under the correspondence principle, the quantum harmonic oscillator has Hamiltonian

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2.$$

So, we want eigenvalues & normalisable eigenstates, such that

$$\hat{\mathcal{H}}|\psi_n\rangle = E_n|\psi_n\rangle, \quad \langle\psi_n|\psi_n\rangle = 1.$$

4.1 Raising & Lowering Operators

Now, let us define some operators, which are combinations of the momentum & position operators;

$$\hat{a} \equiv \frac{1}{\sqrt{2m\hbar\omega}}\left(\hat{p} - im\omega\hat{x}\right), \tag{4.1}$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}\left(\hat{p} + im\omega\hat{x}\right). \tag{4.2}$$

It is clear that $\hat{a}^\dagger$ is adjoint to $\hat{a}$, as both the momentum & position operators are Hermitian. Now, consider the product

$$\begin{aligned}\hat{a}^\dagger\hat{a} &= \frac{1}{2m\hbar\omega}\left(\hat{p} + im\omega\hat{x}\right)\left(\hat{p} - im\omega\hat{x}\right) \\ &= \frac{1}{2m\hbar\omega}\left(\hat{p}^2 - im\omega(\hat{p}\hat{x} - \hat{x}\hat{p}) + m^2\omega^2\hat{x}^2\right),\end{aligned}$$

but, we notice the presence of the commutator $[\hat{p}, \hat{x}] = -i\hbar$. Therefore, the product is

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

So, we see that

$$\begin{aligned}\hbar\omega\hat{a}^\dagger\hat{a} &= \frac{\hat{p}^2}{2m} - \frac{1}{2}\hbar\omega + \frac{1}{2}\omega^2 m\hat{x}^2 \\ &= \hat{\mathcal{H}} - \frac{1}{2}\hbar\omega.\end{aligned}$$

Therefore, we see that we can write the Hamiltonian in terms of our "new operators", as defined above;

$$\hat{\mathcal{H}} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right). \tag{4.3}$$

It is also clear that

$$\hat{a}^\dagger\hat{a} = \frac{\hat{\mathcal{H}}}{\hbar\omega} - \frac{1}{2}. \tag{4.4}$$

The Commutator Let us consider the commutator $\left[\hat{a}, \hat{a}^\dagger\right]$. So,

$$\left[\hat{a}, \hat{a}^\dagger\right] = \frac{1}{2m\hbar\omega}\left[\hat{p} - im\omega\hat{x}, \hat{p} + im\omega\hat{x}\right].$$

The only terms with non-zero contribution are those with both position & momentum. Thus, we see that

$$\left[\hat{a}, \hat{a}^\dagger\right] = \frac{1}{2m\hbar\omega} im\omega\left(\left[\hat{p}, \hat{x}\right] - \left[\hat{x}, \hat{p}\right]\right),$$

which easily gives the result

$$\left[\hat{a}, \hat{a}^\dagger\right] = 1. \tag{4.5}$$

The Eigenstates Let us consider $\hat{\mathcal{H}}\left(\hat{a}^\dagger|\psi\rangle\right)$. So, if we rewrite the Hamiltonian, using (4.3),

$$\hat{\mathcal{H}}\left(\hat{a}^\dagger|\psi\rangle\right) = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \tfrac{1}{2}\right)\hat{a}^\dagger|\psi\rangle.$$

Now, consider the cross-term above. It is

$$\begin{aligned}
\hat{a}^\dagger\hat{a}\hat{a}^\dagger &= \hat{a}^\dagger(\hat{a}\hat{a}^\dagger) \\
&= \hat{a}^\dagger\left(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} - \hat{a}^\dagger\hat{a}\right) \\
&= \hat{a}^\dagger\left(\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} + \hat{a}^\dagger\hat{a}\right) \\
&= \hat{a}^\dagger\left(\left[\hat{a}, \hat{a}^\dagger\right] + \hat{a}^\dagger\hat{a}\right) \\
&= \hat{a}^\dagger\left(1 + \hat{a}^\dagger\hat{a}\right).
\end{aligned}$$

Therefore, we see that we have

$$\hat{\mathcal{H}}\left(\hat{a}^\dagger|\psi\rangle\right) = \hbar\omega\left(\hat{a}^\dagger\left(1 + \hat{a}^\dagger\hat{a}\right) + \frac{1}{2}\hat{a}^\dagger\right)|\psi\rangle.$$

Now, by (4.4), we can rewrite the "middle" bracketed part;

$$1 + \hat{a}^\dagger\hat{a} = \frac{\hat{\mathcal{H}}}{\hbar\omega} + \frac{1}{2},$$

from which we see that

$$\hat{\mathcal{H}}\left(\hat{a}^\dagger|\psi\rangle\right) = \hbar\omega\left(\frac{\hat{a}^\dagger\hat{\mathcal{H}}}{\hbar\omega} + \hat{a}^\dagger\right)|\psi\rangle.$$

Now, as we know that $\hat{\mathcal{H}}|\psi\rangle = E|\psi\rangle$, we therefore see that the above is just

$$\hat{\mathcal{H}}\left(\hat{a}^\dagger|\psi\rangle\right) = (E + \hbar\omega)\,\hat{a}^\dagger|\psi\rangle.$$

Therefore, we see that the Hamiltonian acting upon the state $\hat{a}^\dagger|\psi\rangle$ gives that state, multiplied by a number $(E+\hbar\omega)$. Therefore, $\hat{a}^\dagger|\psi\rangle$ is an eigenstate of the Hamiltonian, with eigenvalue $E + \hbar\omega$.

In a completely analogous way, we find that

$$\begin{aligned}
\hat{\mathcal{H}}\left(\hat{a}|\psi\rangle\right) &= (E - \hbar\omega)\,\hat{a}|\psi\rangle, \\
\hat{\mathcal{H}}\left((\hat{a}^\dagger)^2|\psi\rangle\right) &= (E + 2\hbar\omega)\,(\hat{a}^\dagger)^2|\psi\rangle, \\
\hat{\mathcal{H}}\left(\hat{a}^2|\psi\rangle\right) &= (E - 2\hbar\omega)\,\hat{a}^2|\psi\rangle.
\end{aligned}$$

That is, the Hamiltonian has eigenstates $(\hat{a}^\dagger)^n|\psi\rangle$ with eigenvalues $E + n\hbar\omega$, and eigenstates $\hat{a}^n|\psi\rangle$ with eigenvalues $E - n\hbar\omega$.

For this reason, we call $\hat{a}^\dagger$ the *raising operator*, and its adjoint $\hat{a}$ the *lowering operator*. So, let us state the operators again.

The raising operator is defined as

$$\hat{a}^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}\left(\hat{p} + im\omega\hat{x}\right). \tag{4.6}$$

The lowering operator is defined as

$$\hat{a} \equiv \frac{1}{\sqrt{2m\hbar\omega}}\left(\hat{p} - im\omega\hat{x}\right). \tag{4.7}$$

Preserving Positive Norm Now, consider that $|\chi\rangle = \hat{a}|\psi\rangle$, and that $\langle\chi| = \langle\psi|\hat{a}^\dagger$. Then,

$$\langle\chi|\chi\rangle = \langle\psi|\hat{a}^\dagger\hat{a}|\psi\rangle,$$

using (4.4), we see that this is

$$\langle\chi|\chi\rangle = \langle\psi|\frac{\hat{\mathcal{H}}}{\hbar\omega} - \frac{1}{2}|\psi\rangle = \frac{E}{\hbar\omega} - \frac{1}{2},$$

given that the initial state was normalised, $\langle\psi|\psi\rangle = 1$. Now, the norm of a state should be positive. Therefore, we see that if

$$\langle\chi|\chi\rangle > 0 \quad \Rightarrow \quad \frac{E}{\hbar\omega} - \frac{1}{2} > 0,$$

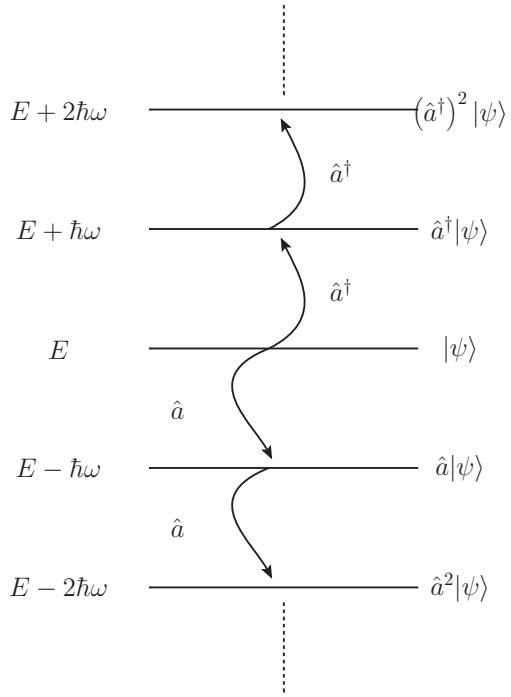

Figure 4.1: The action of operating the raising and lowering operators on a state.

or,

$$\frac{E}{\hbar\omega} > \frac{1}{2}.$$

So, we see that we must have the energy being greater than some value, to preserve positive norm. So, let the minimum energy be

$$E_0 = \frac{\hbar\omega}{2}.$$

We require that there is some state for which

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

then, we call the state the "vacuum state". We denote the vacuum state so that

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

Transferring Between States Suppose we have that

$$|\tilde{n}\rangle = (\hat{a}^\dagger)^n|0\rangle,$$

where $|\tilde{n}\rangle$ is not normalised, and $E_n = E_0 + \hbar\omega$. Then, to find normalisation, we consider that

$$|n\rangle = C(\hat{a}^\dagger)^n|0\rangle,$$

is a normalised state. Then

$$\langle n|n\rangle = |C|^2\langle 0|\hat{a}^n(\hat{a}^\dagger)^n|0\rangle = |C|^2 n!.$$

Therefore, we have that

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle, \quad E_n = (n+\tfrac{1}{2})\hbar\omega$$

as the solution to the eigenvalue problem of the harmonic oscillator.

Consider

$$\begin{aligned}\hat{a}^\dagger\hat{a}|n\rangle &= \left(\frac{\hat{\mathcal{H}}}{\hbar\omega} - \frac{1}{2}\right)|n\rangle \\ &= \left(\frac{(n+\frac{1}{2})\hbar\omega}{\hbar\omega} - \frac{1}{2}\right)|n\rangle \\ &= n|n\rangle.\end{aligned}$$

Thus, if we define the *operator of number of states* $\hat{n} \equiv \hat{a}^\dagger\hat{a}$, then

$$\hat{n}|n\rangle = n|n\rangle.$$

Consider

$$\hat{a}|n\rangle = C|n-1\rangle,$$

then,

$$\langle n|\hat{a}^\dagger\hat{a}|n\rangle = |C|^2\langle n-1|n-1\rangle,$$

and

$$\langle n|\hat{a}^\dagger\hat{a}|n\rangle = n\langle n|n\rangle = 1.$$

Therefore,

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle.$$

Similarly,

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle.$$

Summary of Results

$$\begin{aligned}\left[\hat{a},\hat{a}^\dagger\right] &= 1, && (4.8)\\ \hat{a}^\dagger\hat{a}|n\rangle &= n|n\rangle, && (4.9)\\ \hat{a}|n\rangle &= \sqrt{n}|n-1\rangle, && (4.10)\\ \hat{a}^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle. && (4.11)\end{aligned}$$

4.2 The Vacuum State $\psi_0(x)$

As we previously discussed, there is a "lowest state", for whom when the lowering operator acts upon that state, the answer is zero. That is,

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

We can compute the corresponding wavefunction, $\psi_0(x)$ by usual methods. So, we have that

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

Then, making the product

$$\langle x|\hat{a}|0\rangle = 0,$$

putting the lowering operator into x-representation. Inserting a unity,

$$\sum_{x'} \langle x|\hat{a}|x'\rangle\langle x'|0\rangle = 0.$$

Now, the first term is the matrix element $\langle x|\hat{a}|x'\rangle = \hat{a}_{xx'}$, and the second term is just $\langle x'|0\rangle = \psi_0(x')$. Hence,

$$\sum_{x'} \hat{a}_{xx'}\psi_0(x').$$

Now, we know that

$$\begin{aligned} \hat{a}_{xx'} &= \frac{1}{\sqrt{2m\hbar\omega}} \left(\hat{p} - im\omega\hat{x}\right)_{xx'} \\ &= \frac{1}{\sqrt{2m\hbar\omega}} \left(-i\hbar\frac{d}{dx} - im\omega x\right)\delta_{xx'}. \end{aligned}$$

Therefore, we see that

$$\left(-i\hbar\frac{d}{dx} - im\omega x\right)\psi_0(x) = 0.$$

This easily solves to

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2},$$

where the constant results from normalisation.

Therefore, we have computed the groundstate wavefunction of the quantum harmonic oscillator.

4.3 The General State $\psi_n(x)$

Let us consider how to construct any state, $\psi_n(x)$, of the quantum harmonic oscillator, using the raising operator. That is, we would like to gain an expression for any wavefunction, given the vacuum state; as the raising operator takes us up the states.

Before we begin, we recall the identical result from the "old way" of solving the problem. That is, by solving the Schrodinger equation directly, we find that

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} e^{-\frac{m\omega}{2\hbar}x^2} H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right),$$

where $H_n(y)$ is the n^{th} order Hermite polynomial.

It may already be clear that the raising operator method will be simpler.

Now, we have seen that the state $|n\rangle$ may be constructed from the vacuum state $|0\rangle$ by n applications of the raising operator,

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle.$$

Then, projecting onto x-representation,

$$\begin{aligned}\langle x|n\rangle &= \langle x|\frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle \\ &= \psi_n(x)\end{aligned}$$

inserting a unity,

$$\sum_{x'}\langle x|\frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|x'\rangle\langle x'|0\rangle.$$

Then, this is clearly just

$$\psi_n(x) = \frac{1}{(2m\hbar\omega)^{n/2}}\left(-i\hbar\frac{d}{dx} + im\omega x\right)^n \psi_0(x).$$

Therefore, we have found an expression for the n^{th} state of the quantum harmonic oscillator, by using the raising operators on the vacuum state.

4.4 Eigenstates & Eigenvalues of $\hat{a}$

To compute the eigenstates and eigenvalues of the lowering operator, we must solve the eigenequation

$$\hat{a}|\psi\rangle = \lambda|\psi\rangle, \quad \langle\psi|\psi\rangle = 1.$$

Now, as $\hat{a}$ is clearly not Hermitian, we do not have the immediate restriction that its eigenvalues must be real.

So, projecting the eigenequation into x-representation,

$$\langle x|\hat{a}|\psi\rangle = \lambda\langle x|\psi\rangle = \lambda\psi(x),$$

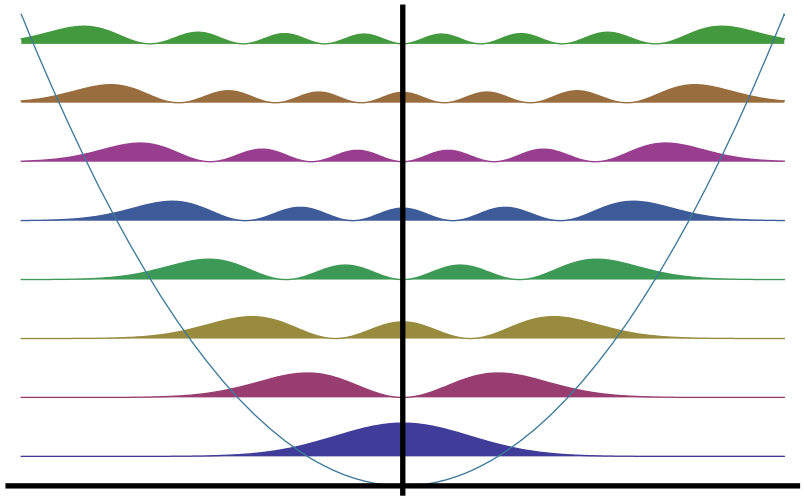

Figure 4.2: The eigenstates of the quantum harmonic oscillator. The "distance up" the vertical axis represents the energy of the state.

inserting a unity,

$$\sum_{x'} \langle x|\hat{a}|x'\rangle\langle x'|\psi\rangle = \lambda\psi(x),$$

which is clearly just

$$\sum_{x'} \hat{a}_{xx'}\psi(x') = \lambda\psi(x).$$

Then, putting in the expression for the operator, we have

$$\frac{1}{\sqrt{2m\hbar\omega}}\left(-i\hbar\frac{d}{dx} + im\omega x\right)\psi(x) = \lambda\psi(x).$$

We can now solve this easily enough. It is simple to get the expression into the form

$$\frac{d\psi}{\psi} = \left(-\frac{m\omega x}{\hbar} + i\lambda\sqrt{\frac{2m\omega}{\hbar}}\right)dx,$$

integrating results in

$$\psi(x) = B.\exp\left(-\frac{m\omega}{2\hbar}x^2 + i\lambda\sqrt{\frac{2m\omega}{\hbar}}x\right).$$

Now, to constrain the possible values of λ (i.e. to the real or complex set of numbers), we must consider the normalisation condition,

$$\int |\psi(x)|^2 = 1.$$

That is, we require a value of λ that will preserve finite norm.

Now, if we consider that the wavefunction is a product of two exponentials; one with argument in $-x^2$, the other in x, and we note that e^{-x^2} decays much quicker than e^x grows (due to the squared-part), then there is no number λ which could pull the growing part above the decaying part. That is, any real or complex number λ works.

Therefore, any number, real or complex, λ is an eigenvalue of the lowering operator.

Let us consider the eigenstates of $\hat{a}$ again, but in energy-representation. So, from the eigenequation, projecting into n-representation,

$$\langle n|\hat{a}|\psi\rangle = \lambda\langle n|\psi\rangle = \lambda\psi_n.$$

Then, inserting a unity,

$$\lambda\psi_n = \sum_m \langle n|\hat{a}|m\rangle\langle m|\psi\rangle.$$

Now, we immediately see that $\langle m|\psi\rangle = \psi_m$. Also, we know that

$$\hat{a}|m\rangle = \sqrt{m}|m-1\rangle.$$

Hence,

$$\lambda\psi_n = \sum_m \sqrt{m}\langle n|m-1\rangle\psi_m,$$

however, due to orthonormality of the energy-states, $\langle n|m-1\rangle = \delta_{n,m-1}$, this is just

$$\sqrt{n+1}\psi_{n+1} = \lambda\psi_n.$$

This easily rearranges to

$$\psi_{n+1} = \frac{\lambda}{\sqrt{n+1}}\psi_n.$$

These are called coherent states.

4.5 Examples

Let us consider a couple of examples; again, they show the ease of solving problems using the raising/lowering operators, rather than the old direct method.

4.5.1 Expected Values of Kinetic Energy & Position

Suppose we wish to know the expected value of kinetic energy,

$$T = \left\langle \frac{p^2}{2m} \right\rangle,$$

using the "old method", this required us to compute the integral

$$\left\langle \frac{p^2}{2m} \right\rangle = \int \psi_n^*(x) \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right) \psi_n(x) dx.$$

For a high-n state, this is very tedious.

Now, from the definitions of $\hat{a}, \hat{a}^\dagger$, we can add and subtract them, to find

$$\hat{p} = \frac{\sqrt{2m\hbar\omega}}{2} \left(\hat{a} + \hat{a}^\dagger \right), \quad \hat{x} = \frac{\sqrt{2m\hbar\omega}}{2im\omega} \left(\hat{a} - \hat{a}^\dagger \right). \tag{4.12}$$

Then, the expected value of the kinetic energy, for a harmonic oscillator in the state $|n\rangle$, is just

$$\begin{aligned} T &= \langle n| \frac{\hat{p}^2}{2m} |n\rangle \\ &= \frac{1}{2m} \left(\frac{\sqrt{2m\hbar\omega}}{2} \right)^2 \langle n| \left(\hat{a} + \hat{a}^\dagger \right)^2 |n\rangle. \end{aligned}$$

Expanding out,

$$T = \frac{\hbar\omega}{4} \langle n| \hat{a}^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + (\hat{a}^\dagger)^2 |n\rangle.$$

Now, we can immediately see that two of these terms will give zero. Consider that the raising operator (on the far right) will create a state $|n+2\rangle$, then, that state will give the product $\langle n|n+2\rangle = 0$. Similarly, the lowering operator on the far left will produce a state $\langle n|n-2\rangle = 0$. Therefore, we are just left with

$$T = \frac{\hbar\omega}{4} \langle n| \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} |n\rangle.$$

Now, if we recall that we have the commutator $\left[\hat{a}, \hat{a}^\dagger\right] = 1$, then we see that we can write

$$\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} = 1 + 2\hat{a}^\dagger\hat{a}.$$

Hence,

$$\begin{aligned} T &= \frac{\hbar\omega}{4} \langle n| 1 + 2\hat{a}^\dagger\hat{a} |n\rangle \\ &= \frac{\hbar\omega}{4} + \frac{\hbar\omega}{2} n \\ &= \frac{\hbar\omega}{2} \left(n + \frac{1}{2} \right) \end{aligned}$$

Therefore, using this, the expected kinetic energy is

$$\begin{aligned} T &= \frac{1}{2} \langle n| \hat{\mathcal{H}} |n\rangle \\ &= \frac{1}{2} E_n. \end{aligned}$$

Therefore, the average kinetic energy, for a quantum harmonic oscillator in the state $|n\rangle$ is $E_n/2$. This result was relatively easy to obtain, and works for any state $|n\rangle$.

The expected value of position is just

$$\langle \hat{x} \rangle = B\langle n|\hat{a} - \hat{a}^\dagger|n\rangle = 0.$$

5 Secondary Quantisation

Pretty much every physical situation has many particles. For example, a cubic metre of air has $\approx 10^{22}$ molecules, and a cubic metre of steel $\approx 10^{23}$. Writing a wavefunction for such a system is formidable. Its form would be something like

$$\psi(x_1, x_2, \ldots, x_{10^{23}}),$$

and is clearly a completely useless quantity to work with.

In quantum mechanics, the situation is simplified by the introduction of the concept of *identical particles*. A few ways to think of identical particles:

- Identical particles are such that under interchange, the physical state of the system is unchanged;
- Identical particles are those which cannot be distinguished by any means.

So, for a 2-particle system, we must make the interchange

$$\psi(x_1, x_2) \longmapsto \psi(x_2, x_1),$$

where we move particle 1 to the position that particle 2 used to have.

Now, the expectation value of a wavefunction is unaffected by the multiplication of a phase $e^{i\alpha}$. That is, $e^{i\alpha}\psi(x)$ and $\psi(x)$ give the same observables. Therefore, to link the interchanged wavefunctions, we suppose that

$$\psi(x_1, x_2) = e^{i\alpha}\psi(x_2, x_1).$$

One can think about this phase shift in the following way. Consider two particles, and that we wish to move them along a line, to interchange their positions. Now, if we make the particle move along the line that joins them directly, then the particle will collide (which is bad). Hence, we make the particle move on trajectories slightly removed from direct. We make them rotate a bit at the point they would collide. That is, we send them on semi-circular trajectories. This is obviously equivalent to rotating the entire system.

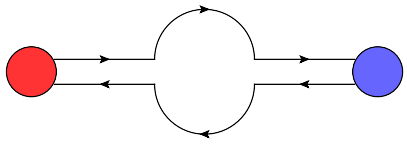

Figure 5.1: Interchanging two particles. Notice that we send the particle along slightly rotated paths: the little semi-circle about the centre- point.

Now, consider that we have interchanged the particles, picking up a phase $e^{i\alpha}$. Then, suppose that we move them back. Thus, we pick up another phase factor. Therefore,

$$\psi(x_1, x_2) = e^{2i\alpha}\psi(x_1, x_2).$$

As we require this to be true, we require that $e^{2i\alpha} = 1$. This is satisfied by the angles $\alpha = 0, \pi$.

Notice then, the two angles give two possibilities for the single-interchange

$$\psi(x_1, x_2) = \psi(x_2, x_1), \quad \psi(x_1, x_2) = -\psi(x_2, x_1).$$

That is, one class of particles are symmetric under particle interchange, and another anti-symmetric.

We call the *symmetric* particles *Bosons*, and the *anti-symmetric* particles *Fermions*.

Notice that for the fermionic case, with two particles in the same place, the interchange is "false",

$$\psi(a, a) = -\psi(a, a) \quad \Rightarrow \quad \psi(a, a) = 0.$$

The Pauli principle is that particles with integer spins are fermions, and particles with half-integer spin ae bosons.

5.1 Bosons & Fermions

As we just discussed, for the two particle case, bosons have totally symmetric wavefunctions, and fermions totally anti-symmetric wavefunctions.

Bose particles Consider the many-particle wavefunction for the Bose case; then, under interchange of any two particles,

$$\psi_B(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_N) = \psi_B(x_1, \ldots, x_j, \ldots, x_i, \ldots, x_N) \quad \forall i, j.$$

Fermi particles Consider the analogous interchange for the Fermionic case,

$$\psi_F(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_N) = (-1)^{Tr}\psi_F(x_1, \ldots, x_j, \ldots, x_i, \ldots, x_N),$$

where $(-1)^{Tr}$ is a sign-factor that we will come to. It essentially figures out how many places the particles had to move.

5.2 Non-interacting Particles

Let us consider N non-interacting particles. Then, the total Hamiltonian is just the sum of the free individual Hamiltonians,

$$\hat{\mathcal{H}}(1, \ldots, N) = \sum_{j=1}^{N} \hat{\mathcal{H}}_0(j),$$

whereby

$$\hat{\mathcal{H}}_0 = \sum_n \varepsilon_n |n\rangle\langle n|.$$

Now, suppose that the wavefunction $\psi_i(x_j)$ denotes that the single particle j is in energy state i. Then, the total wavefunction will be the appropriately symmetrised product of these single particle wavefunctions. That is, for a 2-particle bose-case, the total wavefunction looks like

$$\Psi = \frac{\psi_1(x_1)\psi_n(x_2) + \psi_n(x_1)\psi_1(x_2)}{\sqrt{2}}.$$

That is, the total wavefunction is a (normalised) sum over the possible states of the system (assuming that the particles are either in energy state "1" or "n").

Now, if we start to count up how many particles are in a particular energy state, then we denote n_i as the number of particles, in energy state i. Therefore, for the bose case, we can have n_i as any number; but the fermion case has n_i as only 0 or 1. That is, an energy state (for fermions) either has one or zero particles in it. So, we denote the basis vector

$$|n\rangle = |n_0, n_1, n_2, \ldots, n_j, \ldots\rangle$$

as specifying the number of particles in each state. That is, the occupancy numbers of each state.

5.3 Creation & Destruction Operators

We now introduce the creation and destruction operators. They will allow the number of particles in a system to vary. Now, as the fermion and boson case are so different, we shall discuss them separately.

5.3.1 Bose Case

Now, the general overall wavefunction for non-interacting bosons is

$$\psi(x_1, \ldots, x_N) = \frac{1}{\sqrt{N!}} \sum_{\text{transpositions}} \psi_0(x_1)\ldots\psi_0(x_{n_0})\psi_1(x_{n_0+1})\ldots\psi_1(x_{n_0+n_1})\ldots \\ \ldots\psi_j(x_{\sum_{i=0}^{j-1} n_i})\ldots\psi_j(x_{\sum_{i=0}^{j} n_i})\ldots,$$

where the rather cumbersome notation means: the sum over all transpositions (all combinations) for any number of particles in any one of the states.

Now, let us define the creation and destruction operators.

The creation operator is defined as

$$\hat{a}_j^+ |n_0, \ldots n_j, \ldots\rangle = \sqrt{n_j + 1}|n_1, \ldots, n_j + 1, \ldots\rangle. \tag{5.1}$$

That is, acting the operator $\hat{a}_j^+$ upon a state, increases the number of particles in state j by one.

The destruction operator is defined as

$$\hat{a}_j|n_0, \ldots n_j, \ldots\rangle = \sqrt{n_j}|n_1, \ldots, n_j - 1, \ldots\rangle. \tag{5.2}$$

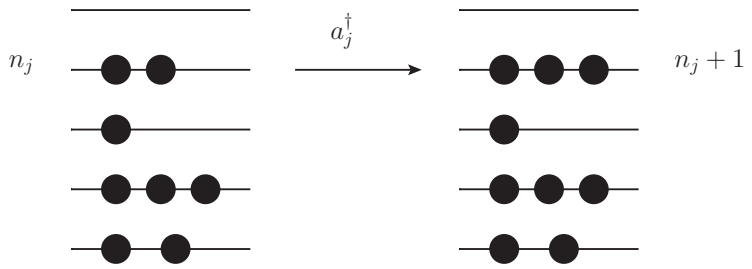

Figure 5.2: The effect of acting the creation operator $\hat{a}_j^+$ upon the system. The number of particles in state j is increased by 1, and the other states remain unchanged. That is, after the action of $\hat{a}_j^+$, there are $n_j + 1$ particles in state j.

Notice that

$$\left(\hat{a}_j\hat{a}_j^+ - \hat{a}_j^+\hat{a}_j\right)|N\rangle$$

will give (reading from far right to left) a decreased number of particles in state j (and a factor of $\sqrt{n_j}$), then the operator $\hat{a}_j^+$ will take that reduced number of particles back up to the beginning value, with a factor of $\sqrt{n_j}$. Then, seeing this for both terms, we see that

$$\left(\hat{a}_j\hat{a}_j^+ - \hat{a}_j^+\hat{a}_j\right)|N\rangle = \left(\sqrt{n_j+1}\sqrt{n_j+1} - \sqrt{n_j}\sqrt{n_j}\right)|N\rangle = |N\rangle.$$

Therefore, we can read off that

$$\hat{a}_j\hat{a}_j^+ - \hat{a}_j^+\hat{a}_j = 1. \tag{5.3}$$

That is, we have the commutator,

$$\left[\hat{a}_j, \hat{a}_j^+\right] = 1. \tag{5.4}$$

In a similar vein, we can see that

$$\left[\hat{a}_i, \hat{a}_j^+\right] = \delta_{ij}, \tag{5.5}$$

and also that

$$\left[\hat{a}_i^+, \hat{a}_j^+\right] = 0, \quad i \neq j.$$

5.3.2 Fermion Case

Here, we must be careful of where we move the "new particle" to. That is, let us create a state,

$$\hat{a}_j^+|N\rangle = |1_j, N\rangle,$$

where we start off by dumping that new state in the start of the ket. We use the notation 1_j to denote an extra particle in state j. Then, we must move that new state up to position j, so that

$$\hat{a}_j^+|n_0, \ldots, n_j, \ldots\rangle = \sqrt{n_j + 1}(-1)^{\sum_{i=0}^{j-1} n_i}|n_0, \ldots, n_j + 1, \ldots\rangle. \tag{5.6}$$

Similarly, the destruction operator dumps the new state in the "first slot", then moves it up to the j^{th} slot. In doing so, a change in sign may be picked up,

$$\hat{a}_j|n_0, \ldots, n_j, \ldots\rangle = \sqrt{n_j}(-1)^{\sum_{i=0}^{j-1} n_i}|n_0, \ldots, n_j - 1, \ldots\rangle. \tag{5.7}$$

These relations differ from the Bose case, due to the sign change. However, both are similar in that a new particle is created in a given state.

Consider

$$\hat{a}_j^+\hat{a}_i^+|N\rangle = \sqrt{n_j + 1}\sqrt{n_i + 1}(-1)^{\sum_{i=0}^{j-1} n_i}|\tilde{N}\rangle,$$

and also

$$\hat{a}_i^+\hat{a}_j^+|N\rangle = \sqrt{n_j + 1}\sqrt{n_i + 1}(-1)^{\sum_{i=0}^{j-1} \tilde{n}_i}|\tilde{N}\rangle.$$

Now, the two expressions are different, with the difference being very subtle. In the first expression, a particle is added to state i, so that the number in that state is $n_i + 1$. This then does something to the overall sign of the state. Then, a particle is added to the state j, so that there are $n_j + 1$ in that state. So, in total, 2 particles were added to the system, with each particle appearing in different states.
The second expression does this the other way round. It adds a particle to state j then to state i. Irrespective of which comes first, i or j, there will be a sign difference between the two methods. Other than the sign, the two methods will produce the same state (i.e. raised the particle number, in two separate states, by two). This is because the "sign factor" wil be raised to a different power, one will be even, one odd. Therefore,

$$\hat{a}_i^+\hat{a}_j^+|N\rangle = -\hat{a}_j^+\hat{a}_i^+|N\rangle.$$

This results in a different sort of commutator. That is, we denote

$$\hat{a}_i^+\hat{a}_j^+ + \hat{a}_j^+\hat{a}_i^+ = 0 \tag{5.8}$$

as

$$\left\{\hat{a}_i^+, \hat{a}_j^+\right\} = 0. \tag{5.9}$$

We call this an "anti-commutator". That is, instead of taking their difference, we take their sum. In a similar way, we can show that

$$\{\hat{a}_i, \hat{a}_j\} = 0, \quad \left\{\hat{a}_i, \hat{a}_j^+\right\} = \delta_{ij}.$$

We use the notation

$$(-1)^{Tr} \equiv (-1)^{\sum_{i=0}^{j-1} n_i},$$

as a transposition factor.

5.4 The Secondary Quantisation Scheme

So, we have seen that we use commutators for bosons, and anti-commutators for fermions. The difference comes when we consider the required anti-symmetry of the fermionic wave-function.

The vacuum state, $|0\rangle$ is that state which contains no particles. Then, the destruction operator acting upon the vacuum state results in

$$\hat{a}_i|0\rangle = 0, \quad \forall i.$$

Therefore, we can construct a state with N particles using the creation operator,

$$|N\rangle = |n_0, n_1 \ldots\rangle = \prod_j \frac{(\hat{a}_j^+)^{n_j}}{\sqrt{n_j}}|0\rangle. \tag{5.10}$$

Hence, we see that the total number of particles is not fixed.

The set of all states $\{|N\rangle\}$ (the set where there are 0 particles, 1 particles, 2 particles etc), is called a *Fock space*. We can transfer between states in the Fock space using the creation and destruction operators. That is, we can write

$$|N\rangle = \hat{Q}|0\rangle, \quad \hat{Q} \equiv \prod_j \frac{(\hat{a}_j^+)^{n_j}}{\sqrt{n_j}}. \tag{5.11}$$

This idea of assigning an operator to a system is called *secondary quantisation*.

States are orthonormal, thus

$$\langle M|\hat{a}_j^+|N\rangle = \sqrt{n_j + 1}\delta_{M,N+1_j}(-1)^{Tr}, \quad \langle M|\hat{a}_j|N\rangle = \sqrt{n_j}\delta_{M,N-1_j}(-1)^{Tr}.$$

The number of particles operator is

$$\hat{n}_j = \hat{a}_j^+\hat{a}_j.$$

5.4.1 Non-interacting Hamiltonian

The Hamiltonian is, as previously stated,

$$\hat{\mathcal{H}} = \sum_j \hat{\mathcal{H}}_0(j).$$

Therefore, inserting two unities,

$$\begin{aligned}\hat{\mathcal{H}} &= \sum_{j,M,N} |M\rangle\langle M|\hat{\mathcal{H}}_0(j)|N\rangle\langle N| \\ &= \sum_{j,M,N} n_j\varepsilon_j|M\rangle\langle M|N\rangle\langle N| \\ &= \sum_{j,N} n_j\varepsilon_j|N\rangle\langle N|.\end{aligned}$$

Thus,

$$\hat{\mathcal{H}} = \sum_N E_N|N\rangle\langle N|, \quad E_n \equiv \sum_j n_j\varepsilon_j.$$

That is, $\hat{\mathcal{H}}$ is diagonal in $|N\rangle$-representation, and E_n is the sum over the number of particles in the single-particle Hamiltonian energy levels ε_j.

Now, as $\hat{n}_j = \hat{a}_j^+\hat{a}_j$ is the particle number operator, we can replace n_j with $\hat{n}_j$ in the Hamiltonian. That is, the Hamiltonian is just the sum over all energy levels times by the number of particles in each energy level. We find the number of particles in each energy level with the $\hat{n}_i$ operator. Therefore,

$$\hat{\mathcal{H}} = \sum_i \varepsilon_i\hat{n}_i = \sum_i \varepsilon_i\hat{a}_i^+\hat{a}_i$$

If there are two-particle interactions, then

$$\hat{\mathcal{H}} = \sum_i \hat{\mathcal{H}}_0(x_i) + \frac{1}{2}\sum_{i,j}\hat{V}(x_i, x_j),$$

which we write, under the second quantisation scheme, as

$$\hat{\mathcal{H}} = \sum_i \varepsilon_i\hat{a}_i^+\hat{a}_i + \frac{1}{2}\sum_{i,k,l,m} V_{ik,lm}\hat{a}_i^+\hat{a}_k^+\hat{a}_l\hat{a}_m.$$

It is important to note the difference between the creation/destruction operators and the raising/lowering operators. The former are able to create particles, whereas the latter merely add energy to particles that are already there.

5.5 Average Number of Particles

For a system with chemical potential μ, at temperature T, with a total number of particles N, then, the mean occupancy of state j is

$$\langle n_j \rangle = \frac{\sum_{k=0}^{\infty} k e^{-\frac{k}{T}(\varepsilon_j - \mu)}}{\sum_{k=0}^{\infty} e^{-\frac{k}{T}(\varepsilon_j - \mu)}},$$

where k will be the number of particles in a given state. The energy of state j is ε_j. To write this, we just used the standard result from the Maxwell-Gibbs relation from statistical mechanics. From this, we define the partition function,

$$Z \equiv \sum_{k=0}^{\infty} e^{-\frac{k}{T}(\varepsilon_j - \mu)} = \frac{1}{1 - e^{-\frac{\varepsilon_j - \mu}{T}}}.$$

Now, notice that

$$T^2 \frac{\partial Z}{\partial T} = \sum_{k=0}^{\infty} k \varepsilon_j e^{-\frac{k}{T}(\varepsilon_j - \mu)}.$$

This only holds for the bosonic case, where we are allowed to take $k = 0, 1, 2, 3 \ldots$.Then, further notice that

$$\langle n_j \rangle = \frac{T^2}{\varepsilon_j} \frac{\partial}{\partial T} \ln Z,$$

then, doing the differential, results in

$$\langle n_j \rangle_B = \frac{1}{e^{\frac{\varepsilon_j - \mu}{T}} - 1}.$$

Therefore, we have used the Maxwell-Gibbs distribution to derive the average number of bosons in energy state ε_j. From this, we have Bose-Einstein condensation, as a consequence of requiring a fixed number of particles as temperature drops and $\mu \to 0$.

For the fermionic case, we take the sum from $k = 0, 1$ only. Hence, we end up with

$$\langle n_j \rangle_F = \frac{1}{e^{\frac{\varepsilon_j - \mu}{T}} + 1}.$$

Now, the point of doing this, within the context of secondary quantisation, is that we can write that

$$\hat{\mathcal{H}} = \sum_i \varepsilon_i \hat{n}_i \quad \Rightarrow \quad \left\langle \hat{\mathcal{H}} \right\rangle = \sum_i \varepsilon_i \langle n_i \rangle,$$

that is, the average energy is

$$\left\langle \hat{\mathcal{H}} \right\rangle = \sum_i \frac{\varepsilon_i}{e^{\frac{\varepsilon_j - \mu}{T}} \pm 1}.$$

5.6 Quasi-particles

Recall the two-particle interaction potential,

$$V = \frac{1}{2} \sum_{i,k,l,m} V_{ik,lm} \hat{a}_i^+ \hat{a}_k^+ \hat{a}_l \hat{a}_m.$$

Now, if the particles are in pairs, we write this as an expansion

$$V = \sum_p w_p \hat{a}_p^+ \hat{a}_{-p}^+ + w_p \hat{a}_p \hat{a}_{-p},$$

so that the Hamiltonian reads

$$\hat{\mathcal{H}} = \sum_p \varepsilon_p \hat{a}_p^+ \hat{a}_p + \sum_p w_p \hat{a}_p^+ \hat{a}_{-p}^+ + w_p \hat{a}_p \hat{a}_{-p}.$$

Now, it is clear that this Hamiltonian is not diagonal. However, let us define a basis in which the Hamiltonian is diagonal. That is, the Hamiltonian will have the form

$$\hat{\mathcal{H}} = \sum_p E_p \hat{b}_p^+ \hat{b}_p,$$

where the operators $\hat{b}_p^+, \hat{b}_p$ satisfy the same anti-commutation relations as $\hat{a}_p^+, \hat{a}_p$;

$$\left\{\hat{a}_p^+, \hat{a}_{p'}\right\} = \delta_{pp'}, \quad \left\{\hat{b}_p^+, \hat{b}_{p'}\right\} = \delta_{pp'}.$$

Then, by using b's rather than a's, we have introduced new "particles", for which the b's are their creation/destruction operators. That is, the operators $\hat{b}_p^+, \hat{b}_p$ correspond to quasi-particles, for which the Hamiltonian is diagonal. The quasi-particles are constructed by some expansion

$$\hat{b}_p = u_p \hat{a}_p + v_p \hat{a}_{-p}^+.$$

6 Symmetries in Quantum Mechanics

Let us consider symmetries, and what consequences they have.

A symmetry is defined as some operation, which when applied to a system, leaves the Hamiltonian of the system unchanged. Then, suppose that O is some symmetry functional, so that

$$O\hat{\mathcal{H}} = \hat{\mathcal{H}}.$$

That O is a functional, rather than an operator (at this stage) means that O changes the things that $\hat{\mathcal{H}}$ is a function of. That is,

$$O : x \mapsto x' = f(x).$$

Then, the symmetry statement is that

$$\hat{\mathcal{H}}\left(f(x)\right) = \hat{\mathcal{H}}(x).$$

Therefore, we see that under the symmetry functional, the Hamiltonian has the same dynamics, in the new coordinate system.

Examples of Symmetry Operations The *time translation* functional,

$$O_T\hat{\mathcal{H}} = \hat{\mathcal{H}} \quad \Rightarrow \quad \hat{\mathcal{H}}(t+T) = \hat{\mathcal{H}}(t),$$

the *space translation*,

$$O_a\hat{\mathcal{H}} = \hat{\mathcal{H}} \quad \Rightarrow \quad \hat{\mathcal{H}}(x+a) = \hat{\mathcal{H}}(x),$$

or the *parity operator*

$$\hat{P}\hat{\mathcal{H}} = \hat{\mathcal{H}} \quad \Rightarrow \quad \hat{\mathcal{H}}(-x) = \hat{\mathcal{H}}(x).$$

Commuting Operators If $\hat{A}$ and $\hat{B}$ are both diagonal in some basis, then $\hat{A}$ and $\hat{B}$ commute. One can see this fairly simply,

$$A_{ij}B_{jk} = a_i\delta_{ij}b_j\delta_{jk} = a_ib_j\delta_{ij} = a_ib_i = b_ia_i.$$

Also, if $\hat{A}$ and $\hat{B}$ commute, then there exists a basis in which they are both diagonal. Similarly, if $\hat{A}, \hat{B}, \hat{C}$ are mutually diagonal in some basis, then they all mutually commute. The converse is also true.

If $\hat{A}$ is a time independent operator which commutes with the Hamiltonian, then the Hamiltonian is conserved. Finally, the set of commuting operators, that commute with the Hamiltonian, provides "good" quantum numbers which are conserved with time.

For example, as the Hamiltonian of a free particle commutes with momentum, $\hat{p}$, then the eigenstates of momentum are able to characterise the Hamiltonian. Also, the Hamiltonian

of many identical particles, as previously discussed, commutes under the operator of particle transposition. Thus, those eigenstates are either symmetric or anti-symmetric, corresponding to either bosons or fermions.

The Hamiltonian of the harmonic oscillator commutes with the parity operator. Therefore, all wavefunctions of the harmonic oscillator are symmetric or anti-symmetric.

Symmetry as an Operator Consider assigning an operator $\hat{O}$ to the functional O. Then, the symmetry operator commutes with the Hamiltonian,

$$\left[\hat{O}, \hat{\mathcal{H}}\right] = 0.$$

Therefore, as the symmetry operator and Hamiltonian commute, they are diagonal in the same basis. Also, therefore, the expectation value of $\hat{O}$ is conserved.

Now, a symmetry operator is not necessarily Hermitian, and therefore will not necessarily give observable quantities.

6.1 The Translation Operator

The translation operator is such that

$$T_a : x^i \mapsto x'^i = x^i + a^i,$$

or,

$$\hat{T}_a \psi(x) = \psi(x + a).$$

We can write the translation operator in a few different forms. Notice that

$$\begin{aligned} e^{a\frac{d}{dx}}\psi(x) &= \sum_{n=0}^{\infty} \frac{a^n}{n!}\frac{d^n}{dx^n}\psi(x) \\ &= \sum_{n=0}^{\infty} \frac{a^n}{n!}\psi^{(n)}(x) \end{aligned}$$

which is just a Taylor expansion of $\psi(x + a)$. Hence,

$$e^{a\frac{d}{dx}}\psi(x) = \psi(x + a).$$

That is, we identify the translation operator with

$$\left(\hat{T}_a\right)_{xx'} = \delta_{xx'} e^{a\frac{d}{dx}}. \tag{6.1}$$

Another way to express the translation operator, is using delta-functions. Recall that

$$\int \delta(y - z) f(z) dz = f(y),$$

then, we could write that

$$\left(\hat{T}_a\right)_{xx'} = \delta(x + a - x'), \tag{6.2}$$

so that

$$\int \left(\hat{T}_a\right)_{xx'} \psi(x')dx' = \psi(x + a).$$

Finally, consider that

$$\hat{T}_a\psi(x) = \chi(x) = \psi(x + a),$$

so that projecting onto bra-ket notation

$$\langle x|\hat{T}_a|\psi\rangle = \langle x|\chi\rangle = \langle x + a|\psi\rangle.$$

Then, working with the far RHS and LHS only, we multiply by $|x\rangle$, and sum,

$$\sum_x |x\rangle\langle x|\hat{T}_a|\psi\rangle = \sum_x |x\rangle\langle x + a|\psi\rangle,$$

we notice that the far LHS is a unity, so that

$$\hat{T}_a|\psi\rangle = \sum_x |x\rangle\langle x + a|\psi\rangle.$$

Therefore,

$$\hat{T}_a = \sum_x |x\rangle\langle x + a|. \tag{6.3}$$

Now, notice that $\hat{T}_a$ is non-Hermitian. That is, one can easily see that

$$\hat{T}_a^\dagger = \sum_x |x + a\rangle\langle x|.$$

Using this, construct

$$\hat{T}_a^\dagger\hat{T}_a = \sum_{x,x'} |x + a\rangle\langle x|x'\rangle\langle x' + a|,$$

the middle term is just a Kronecker-delta, so that

$$\begin{aligned}
\hat{T}_a^\dagger\hat{T}_a &= \sum_{x,x'} |x + a\rangle\delta_{xx'}\langle x' + a| \\
&= \sum_{xx'} \delta_{xx'}|x + a\rangle\langle x' + a| \\
&= \sum_x |x + a\rangle\langle x + a| \\
&= 1.
\end{aligned}$$

Therefore, we see that $\hat{T}_a$ is unitary.

6.1.1 Eigenvalues & Eigenstates of $\hat{T}_a$

Consider solving the eigenequation

$$\hat{T}_a|\psi\rangle = \lambda|\psi\rangle, \quad \langle\psi|\psi\rangle = 1,$$

for λ. That is, we want to solve

$$\psi(x+a) = \lambda\psi(x).$$

So, we take (6.3), and insert two unities,

$$\hat{T}_a = \sum_{x,p,p'} |p'\rangle\langle p'|x\rangle\langle x+a|p\rangle\langle p|.$$

Now, we know that

$$\langle x|p\rangle = P(x) = \frac{1}{(2\pi\hbar)^{n/2}} e^{ipx/\hbar},$$

and hence therefore,

$$\begin{aligned}
\hat{T}_a &= \sum_{x,p,p'} |p'\rangle \frac{1}{(2\pi\hbar)^n} e^{-ip'x/\hbar} e^{ip(x+a)/\hbar} \langle p| \\
&= \sum_{x,p,p'} |p'\rangle\langle p| \frac{1}{(2\pi\hbar)^n} e^{ix(p-p')/\hbar} e^{iap/\hbar} \\
&= \sum_{p,p'} |p'\rangle\langle p| \frac{1}{(2\pi\hbar)^n} \delta(p-p')(2\pi\hbar)^n e^{iap/\hbar} \\
&= \sum_{p} |p\rangle\langle p| e^{iap/\hbar}.
\end{aligned}$$

That is,

$$\hat{T}_a = \sum_{p} |p\rangle\langle p| e^{iap/\hbar}.$$

Hence, we have eigenvalues and eigenstates

$$\lambda = e^{iap/\hbar}, \quad |p\rangle.$$

6.1.2 "The Trick": Relation to Momentum

Now, recall that we showed that the translation operator was unitary. That is,

$$\hat{T}_a^\dagger \hat{T}_a = 1, \quad \forall a.$$

Now, let us take some small δa, and expand in terms of a Taylor series,

$$\hat{T}_{\delta a} \approx 1 + \hat{Q}\delta a, \quad \hat{Q} \equiv \left.\frac{\partial \hat{T}_a}{\partial a}\right|_{a=0}.$$

Similarly, the Hermitian conjugate can be written,

$$\hat{T}_{\delta a}^{\dagger} \approx 1 + \hat{Q}^{\dagger}\delta a.$$

Then, the statement of unitarity is that

$$\hat{T}_a^{\dagger}\hat{T}_a = (1 + \hat{Q}^{\dagger}\delta a)(1 + \hat{Q}\delta a) = 1.$$

So, expanding to first order in δa only,

$$1 + \left(\hat{Q} + \hat{Q}^{\dagger}\right)\delta a = 1$$

which immediately leads us to see that

$$\hat{Q} = -\hat{Q}^{\dagger}.$$

That is, $\hat{Q}$ is *anti-Hermitian.*

Now, let us write that

$$\hat{\pi} = -i\hbar\hat{Q},$$

so that its Hermitian conjugate is

$$\hat{\pi}^{\dagger} = i\hbar\hat{Q}^{\dagger} = -i\hbar\hat{Q} = \hat{\pi}.$$

That is, $\hat{\pi}$ is Hermitian. Furthermore, as $\hat{T}_a$ is conserved, then so is $\hat{Q}$, then so is $\hat{\pi}$. Then, using the representation of $\hat{T}_a$ as

$$\hat{T}_a = e^{a\frac{d}{dx}} \approx 1 + a\frac{d}{dx},$$

we see that we can read off the identification

$$\hat{Q} = \frac{d}{dx},$$

and therefore that

$$\hat{\pi} = -i\hbar\frac{d}{dx} = \hat{p}.$$

This is just the momentum operator. That is, as a consequence of translational invariance of the Hamiltonian operator, we have momentum conservation. Also, recall that we then have

$$\hat{p} = -i\hbar \left.\frac{\partial\hat{T}_a}{\partial a}\right|_{a=0}.$$

We say that $\hat{p}$ are the generators of the translation group.

This has all been for *passive transformations*, whereby we move coordinate systems for a given system. An *active transformation* is one for whom we move the system relative to a fixed coordinate system.

6.2 Generators, Conservation & Gauges

We can generalise the previous discussion.

Consider some symmetry operator $\hat{U}(\alpha)$, which commutes with the Hamiltonian $\hat{\mathcal{H}}(x)$. Then,

$$\hat{U}(\alpha)\hat{\mathcal{H}}(x) = \hat{\mathcal{H}}(x),$$

and

$$\hat{U}(\alpha)\psi(x) = \psi\left(\hat{U}(\alpha)x\right).$$

Also, the symmetry operator is unitary,

$$\hat{U}^\dagger(\alpha)\hat{U}(\alpha) = 1. \tag{6.4}$$

Then, we can expand the operator for small argument,

$$\hat{U}(\delta\alpha) \approx 1 + \delta\alpha \frac{\partial \hat{U}}{\partial \alpha}\bigg|_{\alpha=0}. \tag{6.5}$$

Furthermore, we can define some $\hat{R}$ which is Hermitian and whose expectation value is conserved,

$$\hat{R} \equiv -i\hbar \, \frac{\partial \hat{U}}{\partial \alpha}\bigg|_{\alpha=0}. \tag{6.6}$$

As another example of a symmetry operator, consider the phase operator,

$$\hat{U}_\alpha \equiv e^{i\alpha}, \quad \forall\alpha.$$

This corresponds to adding on a phase shift to the wavefunction, which does nothing to the observables of the state. The associated conserved quantity is

$$\hat{R} \equiv -i\hbar \, \frac{\partial}{\partial \alpha} e^{i\alpha}\bigg|_{\alpha=0} = \hbar.$$

The thing that is actually conserved is the expectation value of $\hat{R}$,

$$\langle\psi|\hat{R}|\psi\rangle = \langle\psi|\hbar|\psi\rangle = \hbar.$$

That is, given an initially normal-wavefunction, the norm is conserved. That is, phase symmetry leads to wavefunction norm conservation.

Now, in adding the phase shift, we have an arbitrary choice of origin. That is, we can choose

$$\alpha' = \alpha - \alpha_0(x).$$

Then,

$$\hat{p} = -i\hbar \frac{d}{dx} e^{-i\alpha_0(x)} \psi(x),$$

therefore, we see that we have some freedom in how we choose this,

$$\hat{p} = -\hbar \frac{d}{dx} + A, \quad A' = A + \frac{\partial \alpha}{\partial x}.$$

That is, we introduce some new field, A, which will allow preservation of symmetries. If the field is a function of position, then the symmetry will be localised, and we call it a *gauge symmetry*. If the symmetry is not a function of position, then the symmetry is *global*.

7 Angular Momentum

Let us consider a rotation, in 3D, about the z-axis, through an angle θ. Then, the change of coordinates are given by

$$\begin{aligned} x' &= x\cos\theta + y\sin\theta, \\ y' &= y\cos\theta - x\sin\theta, \\ z' &= z. \end{aligned}$$

This may be written in matrix form as

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}.$$

So then, consider denoting the transformation operator as $\hat{U}$, then, it is clear from the above that $\hat{U}$ operates on the coordinates only,

$$\tilde{\psi}(x') = \hat{U}\psi(x) = \psi(\hat{U}(x)).$$

That is,

$$\begin{aligned} \tilde{\psi}(x', y', z') &= \psi\left(\hat{U}(x, y, z)\right) \\ &= \psi\left(x\cos\theta + y\sin\theta, y\cos\theta - x\sin\theta, z\right). \end{aligned}$$

Now, it is obvious that the operator $\hat{U}$ is unitary: rotating one way, then back, puts you at the same place you started.

So, given the operator $\hat{U}$, we can expand for small transformation angle, as in the previous section on symmetries. That is, we write

$$\hat{U}(\delta\theta) = 1 - \frac{\hat{R}}{i\hbar}\delta\theta.$$

Also, we use the small angle approximation on the cosine and sine terms,

$$\cos\theta \sim 1, \quad \sin\theta \sim \theta, \quad \theta << 1.$$

Then, the transformation looks like

$$\begin{aligned} \tilde{\psi}(x', y', z') &= \psi\left(\hat{U}(\delta\theta)\right) \\ &= \psi\left(x + y\delta\theta, y - x\delta\theta, z\right). \end{aligned}$$

If we then Taylor expand this,

$$\tilde{\psi}(x', y', z') \approx \psi(x, y, z) + \frac{\partial\psi}{\partial x} y\delta\theta + \frac{\partial\psi}{\partial y}(-x\delta\theta),$$

collecting terms,

$$\begin{aligned}\tilde{\psi}(x',y',z') &\approx \psi(x,y,z)+\left(y\frac{\partial\psi}{\partial x}-x\frac{\partial\psi}{\partial y}\right)\delta\theta \\ &= \left[1+\left(y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y}\right)\delta\theta\right]\psi \\ &= \hat{U}(\delta\theta)\psi.\end{aligned}$$

So, if we compare this with the expansion of the operator, we identify

$$\hat{R}=-i\hbar\left(y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y}\right),$$

which is of course just

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

Now, following our symmetries discussion, $\hat{R}$ is conserved. Therefore, we see that the z-component of angular momentum is conserved.

That is, the rotational symmetry implies conservation of angular momentum. Notice that this is in analogue with norm conservation from phase-shift symmetry, and momentum conservation from translation symmetry.

We can cycle the indices, so that we obtain the full set,

$$\begin{aligned}\hat{L}_x &= y\hat{p}_z-z\hat{p}_y, \\ \hat{L}_y &= z\hat{p}_x-x\hat{p}_z, \\ \hat{L}_z &= x\hat{p}_y-y\hat{p}_x.\end{aligned}$$

Notice that we can group these together into a "vector equation",

$$\hat{\mathbf{L}}=\hat{\mathbf{r}}\times\hat{\mathbf{p}}. \tag{7.1}$$

One may use the language that the $\hat{L}_i$ are the generators for rotations about small angles.

Now, we can fairly easily derive the commutators, using known commutators between position and momentum. So, consider

$$\begin{aligned}\left[\hat{L}_x,\hat{L}_y\right] &= [y\hat{p}_z-z\hat{p}_y,z\hat{p}_x-x\hat{p}_z] \\ &= [y\hat{p}_z,z\hat{p}_x]-[y\hat{p}_z,x\hat{p}_z]-[z\hat{p}_y,z\hat{p}_x]+[z\hat{p}_y,x\hat{p}_z]\,.\end{aligned}$$

Now, the second and third terms are zero. One can see this, as the multiplying coordinate is never the one in the subscript of the momentum. So, we have

$$\left[\hat{L}_x,\hat{L}_y\right]=[y\hat{p}_z,z\hat{p}_x]+[z\hat{p}_y,x\hat{p}_z]\,.$$

Let us explicitly evaluate the first commutator,

$$\begin{aligned}
[y\hat{p}_z, z\hat{p}_x] &= y\,[\hat{p}_z, z\hat{p}_x] \\
&= y\,(\hat{p}_z z\hat{p}_x - z\hat{p}_x\hat{p}_z) \\
&= y\left(-i\hbar\frac{\partial}{\partial z}\,(z\hat{p}_x) - z\hat{p}_x\hat{p}_z\right) \\
&= y\,(-i\hbar\hat{p}_x + z\hat{p}_z\hat{p}_x - z\hat{p}_x\hat{p}_z) \\
&= y\,(-i\hbar\hat{p}_x + z\,[\hat{p}_z, \hat{p}_x]) \\
&= -i\hbar y\hat{p}_x.
\end{aligned}$$

In a very similar way, we can also find that

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

thus giving the commutator

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

That is,

$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\hat{L}_z. \tag{7.2}$$

Again, if we cycle the indices, we find the whole set of commutators,

$$\begin{aligned}
\left[\hat{L}_x, \hat{L}_y\right] &= i\hbar\hat{L}_z, \\
\left[\hat{L}_y, \hat{L}_z\right] &= i\hbar\hat{L}_x, \\
\left[\hat{L}_z, \hat{L}_x\right] &= i\hbar\hat{L}_y.
\end{aligned}$$

We can write this using the totally-antisymmetric Levi-Civita tensor,

$$\left[\hat{L}_a, \hat{L}_b\right] = i\hbar\epsilon_{abc}\hat{L}_c, \quad a, b, c = x, y, z.$$

We shall tend to use indices a, b, c rather than i, j, k, to avoid confusion with the complex number i.

From these, we define

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2,$$

whereby it is obvious (and easily provable) that

$$\left[\hat{L}_i, \hat{L}^2\right] = 0, \quad \forall i = x, y, z.$$

7.1 Eigenstates and Eigenvalues of Angular Momentum

Now, as previously stated in our discussion on commuting operators, that the angular momentum do not commute means that there does not exist a basis in which all $\hat{L}_i$ are diagonal.

So, we shall tend to work with the set of operators that do commute, the biggest set of which are $\hat{L}^2$ with $\hat{L}_i$. For historical reasons, we work with $\hat{L}^2$ and $\hat{L}_z$.

We use the basis $|\lambda, \mu\rangle$, and wish to solve the eigenequations

$$\hat{L}^2|\lambda,\mu\rangle = \lambda^2|\lambda,\mu\rangle, \quad \hat{L}_z|\lambda,\mu\rangle = \mu|\lambda,\mu\rangle;$$

whereby the eigenstates have unit norm, $\langle\lambda,\mu|\lambda,\mu\rangle = 1$.

7.1.1 Ladder Operators

We shall define the ladder operators,

$$\hat{L}_\pm \equiv \hat{L}_x \pm i\hat{L}_y. \tag{7.3}$$

It is clear that $\hat{L}_+$ and $\hat{L}_-$ are adjoint to each other.

So, let us consider the commutator,

$$\begin{aligned}\left[\hat{L}_z, \hat{L}_+\right] &= \left[\hat{L}_z, \hat{L}_x\right] + i\left[\hat{L}_z, \hat{L}_y\right] \\ &= i\hbar\hat{L}_y + \hbar\hat{L}_x \\ &= \hbar\hat{L}_+.\end{aligned}$$

Similarly, one finds that

$$\left[\hat{L}_z, \hat{L}_-\right] = -\hbar\hat{L}_-, \quad \left[\hat{L}_z, \hat{L}_+\right] = \hbar\hat{L}_+. \tag{7.4}$$

Now, consider

$$\begin{aligned}\hat{L}_+\hat{L}_- &= \left(\hat{L}_x + i\hat{L}_y\right)\left(\hat{L}_x - i\hat{L}_y\right) \\ &= \hat{L}_x^2 + \hat{L}_y^2 + i\left[\hat{L}_y, \hat{L}_x\right] \\ &= \hat{L}_x^2 + \hat{L}_y^2 + \hbar\hat{L}_z,\end{aligned}$$

but,

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 \quad \Rightarrow \quad \hat{L}_x^2 + \hat{L}_y^2 = \hat{L}^2 - \hat{L}_z^2,$$

hence, we see that

$$\hat{L}_+\hat{L}_- = \hat{L}^2 - \hat{L}_z^2 + \hbar\hat{L}_z.$$

Rearranging, trivially,

$$\hat{L}^2 = \hat{L}_+\hat{L}_- + \hat{L}_z^2 - \hbar\hat{L}_z.$$

It is also easy to show that a similar result is

$$\hat{L}_-\hat{L}_+ = \hat{L}^2 - \hat{L}_z^2 - \hbar\hat{L}_z.$$

Therefore, as $\hat{L}^2$ and $\hat{L}_z$ commute, so do $\hat{L}_\pm$ and $\hat{L}^2$. That is,

$$\left[\hat{L}_\pm, \hat{L}^2\right] = 0.$$

Now, consider

$$\hat{L}_z\hat{L}_+|\lambda,\mu\rangle,$$

then, by the commutation relation (7.4), we see that this is just

$$\hat{L}_z\hat{L}_+|\lambda,\mu\rangle = \left(\hat{L}_+\hat{L}_z + \hbar\hat{L}_+\right)|\lambda,\mu\rangle.$$

Now, we know the action of $\hat{L}_z$ upon this state, so

$$\begin{aligned}\hat{L}_z\hat{L}_+|\lambda,\mu\rangle &= \left(\hat{L}_+\mu + \hbar\hat{L}_+\right)|\lambda,\mu\rangle \\ &= (\mu+\hbar)\,\hat{L}_+|\lambda,\mu\rangle.\end{aligned}$$

Now, let us write this with some brackets,

$$\hat{L}_z\left\{\hat{L}_+|\lambda,\mu\rangle\right\} = (\mu+\hbar)\left\{\hat{L}_+|\lambda,\mu\rangle\right\}.$$

So, in order for the thing on the RHS to be an eigenstate of $\hat{L}_z$, we then must have that the action of $\hat{L}_+$ upon the state $|\lambda,\mu\rangle$ turns it into a new state $|\lambda,\mu+\hbar\rangle$, which is an eigenstate of $\hat{L}_z$ with eigenvalue $\mu+\hbar$. Therefore,

$$\hat{L}_+|\lambda,\mu\rangle = C_+|\lambda,\mu+\hbar\rangle,$$

and, similarly,

$$\hat{L}_-|\lambda,\mu\rangle = C_-|\lambda,\mu-\hbar\rangle.$$

From this, we say that the action of $\hat{L}_+$ upon a state, increases the projection-number (i.e. the μ bit) by one unit of $\hbar$.

We can find the constant C_+ by requiring the normalisation of $|\lambda,\mu+\hbar\rangle$. So, we have that

$$\hat{L}_+|\lambda,\mu\rangle = C_+|\lambda,\mu+\hbar\rangle,$$

and its Hermitian conjugate,

$$\hat{L}_-\langle\lambda,\mu| = C_+^*\langle\lambda,\mu+\hbar|,$$

so that

$$|C_+|^2\langle\lambda,\mu+\hbar|\lambda,\mu+\hbar\rangle \;=\; \langle\lambda,\mu|\hat{L}_-\hat{L}_+|\lambda,\mu\rangle.$$

That is,

$$\begin{aligned}|C_+|^2 &= \langle\lambda,\mu|\hat{L}_-\hat{L}_+|\lambda,\mu\rangle\\ &= \langle\lambda,\mu|\hat{L}^2-\hat{L}_z^2-\hbar\hat{L}_z|\lambda,\mu\rangle\\ &= \lambda^2-\mu^2-\hbar\mu.\end{aligned}$$

Similarly, one finds that

$$|C_-|^2=\lambda^2-\mu^2+\hbar\mu.$$

Now, it is obvious that we require $|C|\geq 0$. Therefore, we shall say that it is zero for some $\mu_{\rm min},\mu_{\rm max}$. That is,

$$\begin{aligned}\hat{L}_+|\lambda,\mu_{\rm max}\rangle=0 \quad&\Rightarrow\quad \lambda^2-\mu_{\rm max}^2-\hbar\mu_{\rm max}=0,\\ \hat{L}_-|\lambda,\mu_{\rm min}\rangle=0 \quad&\Rightarrow\quad \lambda^2-\mu_{\rm min}^2+\hbar\mu_{\rm min}=0.\end{aligned}$$

Subtracting the two expressions on the right reveals

$$\mu_{\rm min}^2-\mu_{\rm max}^2-\hbar(\mu_{\rm min}+\mu_{\rm max})=0.$$

Or,

$$\mu_{\rm max}=-\mu_{\rm min}.$$

Now, notice that at this maximum value (say),

$$\lambda^2=\mu_{\rm max}(\mu_{\rm max}+\hbar).$$

Furthermore, let us state that $2\mu_{\rm max}=q\hbar$, where q is an integer. Then, $\mu_{\rm max}=-\mu_{\rm min}=\ell\hbar$, where ℓ is an integer or half-integer. Hence, we see that

$$\lambda^2=\ell\hbar^2(\ell+1).$$

Hence, we can now see that

$$\hat{L}^2|\ell,m\rangle = \ell(\ell+1)\hbar^2|\ell,m\rangle, \tag{7.5}$$

$$\hat{L}_z|\ell,m\rangle = m\hbar|\ell,m\rangle, \tag{7.6}$$

$$\hat{L}_\pm|\ell,m\rangle = \sqrt{\ell(\ell+1)-m(m\pm1)}\hbar|\ell,m\pm1\rangle. \tag{7.7}$$

7.1.2 Spherical Harmonics

Consider projecting (7.6) onto the orthogonal coordinate system (θ, ϕ). That is,

$$\langle \theta, \phi | \hat{L}_z | \ell, m \rangle = m\hbar \langle \theta, \phi | \ell, m \rangle,$$

inserting a unity,

$$\sum_{\theta', \phi'} \langle \theta, \phi | \hat{L}_z | \theta', \phi' \rangle \langle \theta', \phi' | \ell, m \rangle = m\hbar \langle \theta, \phi | \ell, m \rangle. \tag{7.8}$$

Now, we define

$$Y_{\ell m}(\theta, \phi) \equiv \langle \theta, \phi | \ell, m \rangle,$$

so that (7.8) reads

$$\sum_{\theta', \phi'} \langle \theta, \phi | \hat{L}_z | \theta', \phi' \rangle Y_{\ell m}(\theta', \phi') = m\hbar Y_{\ell m}(\theta, \phi).$$

Now, we see that by correspondence with previous sections, we write the matrix representation of $\hat{L}_z$ as

$$\left(\hat{L}_z \right)_{\theta\theta'\phi\phi'} = \langle \theta, \phi | \hat{L}_z | \theta', \phi' \rangle,$$

which is just

$$\left(\hat{L}_z \right)_{\theta\theta'\phi\phi'} = -i\hbar \delta_{\theta\theta'} \delta_{\phi\phi'} \frac{\partial}{\partial \phi}.$$

Hence,

$$-i\hbar \frac{\partial}{\partial \phi} Y_{\ell m}(\theta, \phi) = m\hbar Y_{\ell m}(\theta, \phi).$$

Integrating reveals that

$$Y_{\ell m}(\theta, \phi) = P_\ell(\theta) e^{im\phi}.$$

It is also known that

$$\left(\hat{L}^2 \right)_{\theta\theta'\phi\phi'} = -\frac{\hbar^2}{\sin^2 \theta} \left\{ \left(\sin \theta \frac{\partial}{\partial \theta} \right)^2 + \frac{\partial^2}{\partial \phi^2} \right\} \delta_{\theta\theta'} \delta_{\phi\phi'}.$$

So, we say that m is the magnetic (or, projection) quantum number of angular momentum, of the z-component, corresponding to an orbital angular momentum ℓ. There are $2\ell + 1$ values of m for a given ℓ. The magnetic number m has integer values.

Without spin, particles are bosonic.

Up to now, we have only considered orbital angular momentum; which may be thought of as analogous to the motion of the earth about the sun – an orbit. The generic algebra presented here works for spin angular momentum as well.

7.2 Internal Degrees of Freedom

Let us now envisage a particle that is not only determined by its spatial coordinates, but also some internal "coordinates". That is, instead of the wavefunction ψ being a scalar, with argument $\psi(x, y, z)$, let it be a vector,

$$\boldsymbol{\psi} = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} |\psi_1\rangle \\ |\psi_2\rangle \\ \vdots \end{pmatrix}.$$

Now, let us have some operator $\hat{U}$ that does not act upon the (x, y, z)-bit of the wavefunction, but does act upon these extra degrees of freedom. That is, $\hat{U}$ will change the components of ψ,

$$\tilde{\psi} = \hat{U}\psi.$$

Thus, we introduce the *spin* operator, which has the same algebra (and commutators) as orbital angular momentum.

So, the operators are $\hat{S}^2, \hat{S}_x, \hat{S}_y, \hat{S}_z, \hat{S}_\pm$; with the set of eigenvalues/states

$$\hat{S}^2|s, m\rangle = s(s+1)\hbar^2|s, m\rangle, \tag{7.9}$$

$$\hat{S}_z|s, m\rangle = \hbar m|s, m\rangle, \tag{7.10}$$

$$\hat{S}_\pm|s, m\rangle = \sqrt{s(s+1) - m(m \pm 1)}|s, m \pm 1\rangle. \tag{7.11}$$

Thus, s is the spin angular momentum quantum number (or, just spin), with projection m.

One can (inaccurately, but usefully) think of spin as a particle spinning on its axis, much like the rotation of the earth about the poles. This interpretation doesn't quite work as the particles we tend to consider dont always have a "size" about which to rotate.

7.3 Total Angular Momentum

Now, we have seen that orbital and spin angular momentum operators act upon different parts of the wavefunction,

$$\tilde{\boldsymbol{\psi}}(\nu) = \hat{U}_s\boldsymbol{\psi}\left(\hat{U}_o(r)\right),$$

so, we may as well combine these angular momentum operators into a single operator, such that

$$\tilde{\boldsymbol{\psi}}(\nu) = \hat{U}_t\boldsymbol{\psi}(r).$$

That is, we have some new "total operator" $\hat{U}_t$ that incorporates both spin and orbital angular momentum. We call this new operator the *total angular momentum operator*, and denote it $\hat{J}$, where

$$\hat{J} = \hat{L} + \hat{S}. \tag{7.12}$$

The total angular momentum operator uses the same algebra and commutators as both spin and orbital angular momentum:

$$\begin{aligned}
\left[\hat{J}_a, \hat{J}_b\right] &= i\hbar\epsilon_{abc}\hat{J}_c, \quad a,b,c = x,y,z; && (7.13)\\
\hat{J}^2|j,m\rangle &= j(j+1)\hbar^2|j,m\rangle, && (7.14)\\
\hat{J}_z|j,m\rangle &= \hbar m|j,m\rangle, && (7.15)\\
\hat{J}_\pm|j,m\rangle &= \sqrt{j(j+1)-m(m\pm 1)}\hbar|j,m\pm 1\rangle. && (7.16)
\end{aligned}$$

7.3.1 The Scalar State

Suppose we took $j = 0, m = 0$. Then, the state would be $|0,0\rangle$. This state has

$$\hat{J}^2|0,0\rangle = 0, \quad \hat{J}_z|0,0\rangle = 0, \quad \hat{J}_\pm|0,0\rangle = 0;$$

where we easily use the above relations to see this. Clearly, such a state doesn't do much. So, we say that $|0,0\rangle$ is *scalar*.

7.3.2 Spinors

We shall introduce what a "spinor" is, by using an example.

Let us suppose that we take $j = \frac{1}{2}$. Then, the possible values of m are

$$m = -j, -j+1, \ldots, j-1, j \quad \Rightarrow \quad m = -\tfrac{1}{2}, \tfrac{1}{2}.$$

That is, we have two values of m corresponding to this value of j. Then, the two states $|j,m\rangle$ are

$$|\tfrac{1}{2},\tfrac{1}{2}\rangle, \quad |\tfrac{1}{2},-\tfrac{1}{2}\rangle.$$

So, we can also write down that

$$\begin{aligned}
\hat{J}^2|\tfrac{1}{2},\tfrac{1}{2}\rangle &= \tfrac{1}{2}\tfrac{3}{2}\hbar^2|\tfrac{1}{2},\tfrac{1}{2}\rangle = \tfrac{3}{4}\hbar^2|\tfrac{1}{2},\tfrac{1}{2}\rangle,\\
\hat{J}_z|\tfrac{1}{2},\tfrac{1}{2}\rangle &= \tfrac{1}{2}\hbar|\tfrac{1}{2},\tfrac{1}{2}\rangle,\\
\hat{J}_+|\tfrac{1}{2},\tfrac{1}{2}\rangle &= \sqrt{\tfrac{1}{2}\tfrac{3}{4}-\tfrac{1}{2}\tfrac{3}{4}}\hbar|\tfrac{1}{2},\tfrac{1}{2}+1\rangle = 0,\\
\hat{J}_-|\tfrac{1}{2},\tfrac{1}{2}\rangle &= \sqrt{\tfrac{1}{2}\tfrac{3}{4}+\tfrac{1}{2}\tfrac{1}{4}}\hbar|\tfrac{1}{2},-\tfrac{1}{2}\rangle = \hbar|\tfrac{1}{2},-\tfrac{1}{2}\rangle,
\end{aligned}$$

with all other relations being trivial (and tedious) to write.

So, let us introduce some notation,

$$|\tfrac{1}{2},\tfrac{1}{2}\rangle \equiv |\uparrow\rangle, \quad |\tfrac{1}{2},-\tfrac{1}{2}\rangle \equiv |\downarrow\rangle. \qquad (7.17)$$

Hence, we see that

$$\hat{J}_+|\uparrow\rangle = 0, \quad \hat{J}_-|\uparrow\rangle = \hbar|\downarrow\rangle,$$
$$\hat{J}_+|\downarrow\rangle = \hbar|\uparrow\rangle, \quad \hat{J}_-|\downarrow\rangle = 0.$$

Now, we further notate these "upstates" and "downstates" as

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{7.18}$$

So, we can construct any state from a linear combination of these,

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \alpha \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

again, we give an alternative way of notating this,

$$|\chi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle.$$

Now, the components, α, β may be complex. In this case, the state $|\chi\rangle$ is called a *spinor*. A spinor is just the name given to state vectors, in a complex vector space. The states are normalised,

$$\langle\chi|\chi\rangle = |\alpha|^2 + |\beta|^2 = 1.$$

Now, the operators $\hat{J}_i$ are generated using the Pauli-spin matrices,

$$\hat{J}_i = \frac{\hbar\hat{\sigma}_i}{2}, \tag{7.19}$$

where the $\hat{\sigma}_i$ are given by

$$\hat{\sigma}_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}_z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{7.20}$$

The spin matrices can easily be shown to conform to the commutation relations

$$[\hat{\sigma}_a, \hat{\sigma}_b] = 2i\epsilon_{abc}\hat{\sigma}_c, \tag{7.21}$$

and equally as easy to the anti-commutation relations

$$\{\hat{\sigma}_a, \hat{\sigma}_b\} = 2\delta_{ab}. \tag{7.22}$$

Although we haven't gone into the details of generators of groups at all, it is worth noting that

$$e^{i\hat{\sigma}_a\hat{n}_a}$$

is the generator of the group of rotations in 3D, where $\hat{n}_a$ is the unit vector.

7.4 Multiplication of Angular Momenta

Now, we know that from the previous sections discussion, for a given value of the total angular momentum quantum number j there are $2j+1$ values of the projection quantum number m. The eigenstates of angular momentum are $|j,m\rangle$. Now, suppose we have two particles, each with their own angular momentum states, what is the resultant angular momentum? That is, how can we compute the product of two angular momentum states $|j_1,m_1\rangle$ and $|j_2,m_2\rangle$? What is the total J and total M of the new system?

Now, the total angular momentum operators are defined to be the sum

$$\hat{J}_{tot} = \hat{J}_1 + \hat{J}_2, \quad \hat{J}_{z_{tot}} = \hat{J}_{z_1} + \hat{J}_{z_2}.$$

However, the square is not just the sum of the squares, as

$$\hat{J}^2_{tot} = \hat{J}^2_1 + \hat{J}^2_2 + \hat{J}_1\hat{J}_2 + \hat{J}_2\hat{J}_1.$$

This complicates things somewhat!

Now, let us use the notation that

$$|j_1,m_1;j_2,m_2\rangle = |j_1,m_1\rangle|j_2,m_2\rangle.$$

Hence, as there are $(2j_i+1)$ m_i states per system, there are $(2j_1+1)(2j_2+1)$ states for the total system. So, the projection operator is fairly easy to compute,

$$\begin{aligned}\hat{J}_{z_{tot}}|j_1,m_1;j_2,m_2\rangle &= \left(\hat{J}_{z_1}+\hat{J}_{z_2}\right)|j_1,m_1\rangle|j_2,m_2\rangle \\ &= \hbar(m_1+m_2)|j_1,m_1\rangle|j_2,m_2\rangle \\ &= \hbar(m_1+m_2)|j_1,m_1;j_2,m_2\rangle.\end{aligned}$$

The total angular momentum is not so easy to find. Basically, the answer is that a linear combination of states is produced, where the possible values of total angular momentum are

$$J = |j_1-j_2|, |j_1-j_2+1|, \ldots, |j_1+j_2|.$$

The coefficients of the linear combinations are known as the Clebsh-Gordan coefficients,

$$|j_1,m_1;j_2,m_2\rangle = \sum_{J,M}\langle J,M|j_1,m_1;j_2,m_2\rangle|J,M\rangle, \quad M \equiv m_1+m_2.$$

These coefficients are messy, and are generally "looked up" if one needs to know them. The Clebsh-Gordan coefficients are orthogonal.

8 Charged Particle in EM Field

Recall the Lorentz force on a charged particle,

$$\mathbf{F} = q\mathbf{E} + \frac{q}{c}\mathbf{v} \times \mathbf{B},$$

where we shall be using cgs units. The electric and magnetic fields relate to the potentials via

$$\mathbf{E} = -\nabla\phi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}, \quad \mathbf{B} = \nabla \times \mathbf{A}.$$

Notice that by introducing these potentials, we have reduced the number of parameters from 6 (in 3 components of the fields) to 4 (in the 3 of the vector, and 1 of scalar potential). Now, the potentials are not uniquely defined, and are free up to the choice of gauge transformation,

$$\phi' = \phi + \frac{1}{c}\frac{\partial \chi}{\partial t}, \quad \mathbf{A}' = \mathbf{A} - \nabla\chi,$$

where χ is an arbitrary function. We use the gauge fixing of the Coulomb gauge to state that

$$\nabla \cdot \mathbf{A} = 0,$$

so that in using this, the fields do not change.

8.1 Pauli Hamiltonian

Let us postulate the Hamiltonian

$$\hat{\mathcal{H}} = \frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{q}{c}\mathbf{A}\right)^2 + q\phi - \frac{gq}{2mc}\hat{\mathbf{S}} \cdot \mathbf{B}, \tag{8.1}$$

where $\hat{\mathbf{S}}$ are the spin matrices, and g the gyromagnetic ratio. This is the non-relativistic Hamiltonian of a particle with charge q in an electromagnetic field, with magnetic field $\mathbf{B}$, vector and scalar potential $\mathbf{A}, \phi$. We call it the *Pauli Hamiltonian.*

The part in the Hamiltonian,

$$\hat{\mathbf{p}} - \frac{q}{c}\mathbf{A}$$

is said to be of the form *minimal coupling*, and is an analogue of the covariant derivative.

The interaction of the charged particle with the electric field is described by the

$$q\phi$$

term. The interaction with the magnetic field is described by the

$$-\frac{gq}{2mc}\hat{\mathbf{S}} \cdot \mathbf{B}$$

term.

The gauge transformation previously stated gives freedom in changing the phase of the wavefunction,

$$\tilde{\psi}(\mathbf{r},t) = \psi(\mathbf{r},t)e^{\frac{iq}{\hbar c}\chi(\mathbf{r},t)}.$$

Now, it is common to notate the magnetic interaction term in terms of the magnetic moment,

$$\frac{gq}{2mc}\hat{\mathbf{S}}\cdot\mathbf{B} = \hat{\boldsymbol{\mu}}\cdot\mathbf{B}.$$

8.1.1 Spin Dynamics

The Schrodinger equation, as always, is given by

$$i\hbar|\dot{\psi}\rangle = \hat{\mathcal{H}}|\psi\rangle.$$

Now, suppose we have a particle in a homogeneous magnetic field (i.e. the magnetic field is constant in space). Then, we can separate the wavefunction into its space and spin parts,

$$|\psi\rangle = |\psi(\mathbf{r})\rangle|\eta\rangle.$$

Each "type" of state is normalised,

$$\langle\psi(\mathbf{r})|\psi(\mathbf{r})\rangle = 1, \quad \langle\eta|\eta\rangle = 1.$$

The spin state, in general, has n components α_n, whereby

$$|\eta\rangle = \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix}, \quad \sum_{i=1}^{n}|\alpha_i|^2 = 1.$$

Let us consider a spin-$\frac{1}{2}$ electron. We shall use the spin basis discussed in the previous section. The spin operator, for such a system, is just formed from the Pauli-matrices,

$$\hat{\mathbf{S}} = \frac{\hbar}{2}\hat{\boldsymbol{\sigma}}.$$

Hence, such a system has its wavefunction written as

$$|\psi\rangle = \begin{pmatrix} |\psi_\uparrow\rangle \\ |\psi_\downarrow\rangle \end{pmatrix}.$$

For an electron, $g = 2, q = e$. Using this, and writing the spin operator as the Pauli matrices, we rewrite the Pauli Hamiltonian (8.1) as

$$\hat{\mathcal{H}} = \frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}\right)^2 + e\phi - \frac{e\hbar}{2mc}\hat{\boldsymbol{\sigma}}\cdot\mathbf{B}$$

Introducing the *Bohr magneton*,

$$\mu_B \equiv \frac{e\hbar}{2mc},$$

the Pauli Hamiltonian becomes

$$\hat{\mathcal{H}} = \frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}\right)^2 + e\phi - \mu_B \hat{\boldsymbol{\sigma}} \cdot \mathbf{B}.$$

Let us now use this Hamiltonian to write the Schrodinger equation for a particle in a homogeneous magnetic field. We recall that we separate the wavefunction into its space and spin parts, so that the Schrodinger equation is written as two equations:

$$i\hbar|\dot{\psi}(\mathbf{r})\rangle = \left[\frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}\right)^2 + e\phi\right]|\psi(\mathbf{r})\rangle, \tag{8.2}$$

$$i\hbar|\dot{\eta}\rangle = -\mu_B \hat{\boldsymbol{\sigma}} \cdot \mathbf{B}|\eta\rangle. \tag{8.3}$$

The spin equation describes the spin dynamics of a charged spin-$\frac{1}{2}$ particle in a magnetic field.

Spin Precession Consider a charged spin-$\frac{1}{2}$ particle magnetic field $\mathbf{B} = (0, 0, B_z)$, where B_z is constant. Then, the spin dynamics equation becomes

$$i\hbar\frac{d}{dt}|\eta\rangle = -\mu_B B_z \hat{\sigma}_z|\eta\rangle.$$

To avoid confusion, let us write this equation down explicitly, in terms of matrices;

$$i\hbar\begin{pmatrix} \dot{\eta}_\uparrow \\ \dot{\eta}_\downarrow \end{pmatrix} = -\mu_B B_z \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} \eta_\uparrow \\ \eta_\downarrow \end{pmatrix}.$$

Expanding out the equations, we get

$$i\hbar\frac{d\eta_\uparrow}{dt} = -\mu_B B_z \eta_\uparrow, \tag{8.4}$$

$$i\hbar\frac{d\eta_\downarrow}{dt} = \mu_B B_z \eta_\downarrow. \tag{8.5}$$

These equations are easily integrated, and solved to give

$$\eta_\uparrow = \eta_\uparrow(0)e^{i\Omega t},$$

$$\eta_\downarrow = \eta_\downarrow(0)e^{-i\Omega t}, \quad \Omega \equiv \frac{\mu_B B_z}{\hbar}.$$

These equations describe the precession of an initial spin state. That is, the spins precess with angular frequency Ω.

8.2 Phenomenology

Here we shall discuss some interesting effects that quantum theory predicts.

8.2.1 The Aharonov–Bohm Effect

Consider the change in phase of a charged particle, upon moving along some path γ

$$\varphi = \frac{1}{\hbar}\int_\gamma \left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)\cdot d\mathbf{r},$$

or, just pulling out the magnetic part,

$$\varphi_{mag} = -\frac{q}{\hbar c}\int_\gamma \mathbf{A}\cdot d\mathbf{r}.$$

Now, consider that the particle moves along two paths γ_1 and γ_2, consecutively, in the presence of a vector potential,

$$\Delta\varphi_{mag} = -\frac{q}{\hbar c}\left(\int_{\gamma_1}\mathbf{A}\cdot d\mathbf{r} - \int_{\gamma_2}\mathbf{A}\cdot d\mathbf{r}\right).$$

We see that via Stokes' theorem, this is just the flux of $\mathbf{B}$ through the surface bound by the contour $\gamma_1 + \gamma_2$;

$$\Delta\varphi_{mag} = -\frac{q}{\hbar c}\oint \mathbf{B}\cdot\hat{\mathbf{n}}dS,$$

where $\hat{\mathbf{n}}$ is the unit normal of the surface element dS. Let us write this flux as

$$\Phi \equiv \oint \mathbf{B}\cdot\hat{\mathbf{n}}dS,$$

so that the phase change is

$$\Delta\varphi_{mag} = -\frac{q}{\hbar c}\Phi. \tag{8.6}$$

Hence, we see that as a particle completes its motion about a closed loop, there is a phase change of the wavefunction, and a magnetic flux associated.

This effect can be experimentally "seen" by putting a solenoid in a system. Consider that electrodynamic theory says that there is no magnetic field outside of a solenoid, but the vector potential does exist outside of the solenoid. That is, for a magnetic field passing through an area A, there will be no magnetic field outside of the solenoid, but there will be an angular component of the vector potential,

$$A_\theta = \frac{\Phi}{2\pi r},$$

where Φ is the magnetic flux through the solenoid, and r the distance from the centre of the solenoid.

Now, using the standard Youngs' double-slit experimental setup (using electrons), as one moves along the screen, one sees an interference pattern. The interference pattern is due to the slightly different path lengths of the two beams, as they come through the slits. As a function of the difference in path lengths, the interference pattern observed is

$$|\psi|^2 \sim 2|\psi_0|^2 \left[1 + \cos\left(\frac{|p|(L_1 - L_2)}{\hbar}\right)\right].$$

That is, one will see a sequence of light and dark spots, as the path length sweeps through integer and half-integer multiples of 2π. That is,

$$\begin{aligned} |p|(L_1 - L_2) = 2\pi m\hbar \quad &\Rightarrow \quad \text{constructive,} \\ |p|(L_1 - L_2) = (2\pi m + \pi)\,\hbar \quad &\Rightarrow \quad \text{destructive.} \end{aligned}$$

We now modify the setup, so that between the slits and the screen is the solenoid, with a magnetic field through it. It is important to note again that there will not be any magnetic field outside of the solenoid, but there will be a component of the magnetic vector potential.

Now, the phase of the two electron beams will be different from the no-solenoid case. That is, there will be an additional phase shift, due to the vector potential being generated, by the solenoid. This extra phase shift has the observable effect of shifting the interference pattern along. The phase difference, for constructive interference, without the solenoid, was

$$\Delta\varphi_0 = 2\pi m,$$

and with solenoid is now

$$\Delta\varphi = \Delta\varphi_0 - \frac{q}{\hbar c}\Phi.$$

We can basically now state that the Aharonov–Bohm effect is an interference effect which appears when charged particles pass through a region of space with zero magnetic field, but non-zero vector potential. What this means is that the vector potential is more fundamental than the field itself.

8.2.2 Flux Quantisation

Suppose that charged particles are forced to move around a circle. Then, if there is a magnetic field present, there will be a phase shift after every revolution (as we have just seen). If the phase difference is $2\pi n$, the particles will not "notice" the shift, as everything will be as it was when they first went round. However, if the phase shift is not $2\pi n$, then after many revolutions the particles wavefunctions will interfere and eventually cancel out.

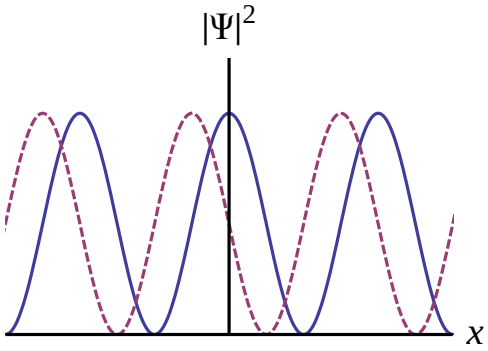

Figure 8.1: The shift in interference pattern observed, with solenoid: The Aharonov–Bohm effect. Undashed is no-solenoid, dashed has the solenoid.

We saw that the phase shift, due to magnetic flux, is

$$\Delta\varphi_{mag} = \frac{q\Phi}{\hbar c}.$$

So, this must be an integer number of 2π's, for the wavefunctions to not-cancel. That is, we have

$$\Delta\varphi_{mag} = \frac{q\Phi}{\hbar c} = \begin{cases} 2\pi n & \Rightarrow \text{ constructive} \\ 2\pi n + \epsilon & \Rightarrow \text{ destructive.} \end{cases}$$

Hence, we see that the properties of the system will change perdiodically, due to the presence of the magnetic flux. Hence, for this not to happen, we require the quantisation of the flux of the magentic field, such that

$$\Phi = \frac{2\pi n\hbar c}{q}.$$

8.2.3 Fractional Statistics

Let us consider a 2D slab of electrons. To construct such a slab, one could consider sandwiching a very thin slice of conductor between two insulators. Then, motion of the electrons would effectively be confined to the $x-y$-plane.

Now, put a solenoid through the 2D slab, so that the electrons will orbit the solenoid. The Hamiltonian for such a system can be written, from the Pauli Hamiltonian,

$$\hat{\mathcal{H}} = \frac{1}{2m}\left[\left(p_r - \frac{e}{c}A_r\right)^2 + \left(p_\theta - \frac{e}{c}A_\theta\right)^2\right] + \hat{U}(r).$$

We know that, from our previous discussions,

$$A_\theta = \frac{\Phi}{2\pi r}.$$

Basically, the solution to the Schrodinger equation takes on the form

$$\psi_m(r,\theta) = R_m(r)e^{\left[i\left(m+\frac{e\Phi}{\hbar c}\right)\theta\right]},$$

where we must have the quantisation rule

$$m + \frac{e\Phi}{\hbar c} = n,$$

where n is an integer.

Now, suppose we put two solenoids through the slabs. There will be (say) an electron orbiting each solenoid. Now, suppose we exchange the electrons, by rotating the system (let us leave the solenoids where they are). The electrons will pick up a phase shift, because they will be cutting the flux lines,

$$\Delta\varphi \sim e^{i\alpha}, \quad \alpha \equiv \frac{e\Phi}{\hbar c}.$$

Basically, if the electrons pick up a phase shift of -1, they are fermions. However, this need not be the case. That is, upon the exchange of particles, we can make the electrons pick up an arbitrary phase shift.

This is called fractional statistics, whereby particles can have any phase shift.

It is also interesting to note that this effect is not possible in a 3D gas of electrons. The reason for the existence of fractional statistics in 2D, and not 3D, is due to the topology of the group of rotations (i.e. pretty complicated!). Consider in 3D, two particles in distinct locations. We can exchange the particles by making them move on tracjectories between the locations. We can send one particle along one trajectory, and the other on a trajectory rotated a little-bit-upwards from the first trajectory. Infact, we can rotate the second trajectory all the way round, until a circle is formed. Now, it is very important to note that every one of these rotations is still within the 3D space (it is fairly obvious, but important). That is, we say that the 3D group of rotations in simply connected. This is not the case in 2D: one cannot rotate "upwards" in 2D, remaining in 2D! That is, the 2D group of rotations is not simply connected.

8.2.4 Landau Orbitals

Suppose we write the Pauli Hamiltonian as

$$\hat{\mathcal{H}} = \frac{1}{2m}\left(p_x + \frac{e}{2c}B_y\right)^2 + \frac{1}{2m}\left(p_y - \frac{e}{2c}B_x\right)^2,$$

where there is obviously a vector potential

$$\mathbf{A} = (-\tfrac{1}{2}B_y, \tfrac{1}{2}B_x, 0).$$

So, suppose we want to find the energy levels of such a system, we would then want to solve

$$\hat{\mathcal{H}}|\psi\rangle = E|\psi\rangle.$$

Now, the Hamiltonian is of the form that suggests we write something like

$$a^2 + b^2 = (a + ib)(a - ib),$$

where we shall write

$$\begin{aligned}
\hat{a} &= \frac{1}{2\sqrt{eB/2c\hbar}}\left(p_x + \frac{e}{2c}B_y + i\left(p_y - \frac{e}{2c}B_x\right)\right), \\
\hat{a}^\dagger &= \frac{1}{2\sqrt{eB/2c\hbar}}\left(p_x + \frac{e}{2c}B_y - i\left(p_y - \frac{e}{2c}B_x\right)\right).
\end{aligned}$$

Hence, we have something very similar to our harmonic oscillator problem of a few sections ago. That is, we have commutation relation and Hamiltonian

$$\left[\hat{a}, \hat{a}^\dagger\right] = 1, \quad \hat{\mathcal{H}} = \hbar\omega_B(\hat{a}^\dagger\hat{a} + \tfrac{1}{2}).$$

Thus, an orbital that oscillates.

8.3 Quantum Theory of Radiation

Consider the Pauli Hamiltonian, with interaction term,

$$\hat{\mathcal{H}} = \frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}\right)^2 + e\phi - \mu_B\hat{\boldsymbol{\sigma}}\cdot\mathbf{B} + \hat{\mathcal{H}}_{EM},$$

where $\mathbf{A}$ and $\mathbf{E}$ are classical fields. We call $\hat{\mathcal{H}}$ the semi-classical Hamiltonian. If we open out the bracket on this Hamiltonian, we see that we can write it as

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + e\phi - \frac{e}{mc}\mathbf{A}\cdot\hat{\mathbf{p}} - \mu_B\hat{\boldsymbol{\sigma}}\cdot\mathbf{B} + \frac{e^2}{2mc^2}\mathbf{A}^2 + \hat{\mathcal{H}}_{EM}.$$

The first thing to note, is that we have allowed $\hat{\mathbf{p}}$ and $\mathbf{A}$ to commute. This is because of the Coulomb gauge $\nabla\cdot\mathbf{A} = 0$. We can write this Hamiltonian as a sum of "smaller" ones,

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_a + \hat{\mathcal{H}}_I + \hat{\mathcal{H}}_{EM},$$

where the *atomic Hamiltonian* is

$$\hat{\mathcal{H}}_a \equiv \frac{\hat{p}^2}{2m} + e\phi,$$

and the *interaction Hamiltonian*

$$\hat{\mathcal{H}}_I \equiv -\frac{e}{mc}\mathbf{A}\cdot\hat{\mathbf{p}} - \mu_B\hat{\boldsymbol{\sigma}}\cdot\mathbf{B} + \frac{e^2}{2mc^2}\mathbf{A}^2.$$

The electromagnetic Hamiltonian $\hat{\mathcal{H}}_{EM}$ is that of the electromagnetic field.

If the "value of" the atomic Hamiltonian is much greater than that of the interaction Hamiltonian, then we can write its Schrodinger equation,

$$\hat{\mathcal{H}}_a|N_a\rangle = E_n|N_a\rangle, \quad |N_a\rangle = |n, j, m\rangle;$$

where we have used the atomic states $|N_a\rangle$. The quantum number n is the principle (or, radial) quantum number, j the angular momentum and m the projection (or magnetic) quantum number.

Transitions are described by the matrix element

$$V_{N'N} = \langle N'|\hat{\mathcal{H}}_I|N\rangle.$$

The Fermi golden rule is

$$w_{d\Omega} = \frac{2\pi}{\hbar}\left|V_{N'N}\right|^2 \rho(E_N - E_{N'})\delta(E_N - E_{N'} - \hbar\omega)d\Omega, \tag{8.7}$$

where $w_{d\Omega}$ is the transition probability for a given elemental solid angle; ρ is the density of states.

As a small aside, consider the term

$$-\frac{e}{mc}\mathbf{A}\cdot\hat{\boldsymbol{p}} = -\frac{e}{mc}\mathbf{A}\cdot\frac{d\mathbf{x}}{dt}m,$$

which we can write as

$$-\frac{e}{c}\mathbf{A}\cdot\frac{d\mathbf{x}}{dt} = -\frac{e}{c}\frac{d}{dt}\left(\mathbf{A}\cdot\mathbf{x}\right) + \frac{e}{c}\mathbf{x}\cdot\frac{d\mathbf{A}}{dt}.$$

Now, if the fields are periodic, the first term on the RHS is zero. Now, in vacuum,

$$\mathbf{E} = -\frac{1}{c}\frac{d\mathbf{A}}{dt}.$$

Hence,

$$-\frac{e}{mc}\mathbf{A}\cdot\hat{\boldsymbol{p}} = -e\mathbf{x}\cdot\mathbf{E}.$$

Now, a charge multiplied by the field is just the electric dipole, so that

$$-\frac{e}{mc}\mathbf{A}\cdot\hat{\boldsymbol{p}} = -\mathbf{E}\cdot\mathbf{d}.$$

Hence, we see that part of the interaction Hamiltonian can be rewritten using this, as

$$-\frac{e}{mc}\mathbf{A}\cdot\hat{\boldsymbol{p}} - \mu_B\hat{\boldsymbol{\sigma}}\cdot\mathbf{B} \longmapsto -\mathbf{E}\cdot\mathbf{d} - \hat{\boldsymbol{\mu}}\cdot\mathbf{B},$$

which is a semi-classical expression.

Let us get back to a quantum mechanical approach.

Recall Maxwell's equations,

$$\nabla \cdot \mathbf{E} = 4\pi\rho, \quad \nabla \times \mathbf{E} = -\tfrac{1}{c}\dot{\mathbf{B}},$$
$$\nabla \cdot \mathbf{B} = 0, \quad \nabla \times \mathbf{B} = \tfrac{4\pi}{c}\mathbf{J} + \tfrac{1}{c}\dot{\mathbf{E}},$$

and the relations of the fields to the potentials,

$$\mathbf{E} = -\frac{1}{c}\dot{\mathbf{A}} - \nabla\phi, \quad \mathbf{B} = \nabla \times \mathbf{A}.$$

Now, taking the divergence of the first expression,

$$\nabla \cdot \mathbf{E} = -\frac{1}{c}\frac{\partial}{\partial t}\nabla \cdot \mathbf{A} - \nabla^2\phi = 4\pi\rho,$$

where we have used the first Maxwell equation. Now, if we use the *Coulomb gauge*, $\nabla \cdot \mathbf{A} = 0$, this reduces to

$$-\nabla^2\phi = 4\pi\rho,$$

which is a wave equation, with static (Coulomb) solution

$$\phi(\mathbf{x}, t) = -\int \frac{\rho(\mathbf{x}', t)}{|\mathbf{x}' - \mathbf{x}|}dx'.$$

Thus, for a given distribution of charge, one can find the scalar potential, and thus reducing the number of free parameters in the potentials by one.

The vector potential may be written as a spherical wave,

$$\mathbf{A} = \mathbf{A}_0 e^{i\mathbf{k}\cdot\mathbf{x}},$$

and its divergence is zero, by the Coulomb gauge,

$$\nabla \cdot \mathbf{A} = \mathbf{k} \cdot \mathbf{A} = 0.$$

Therefore, the direction of the vector potential and direction of propagation are always perpendicular. That is, there is no parallel component between the wavevector $\mathbf{k}$ and the vector potential $\mathbf{A}$.

In free space, the wave equation becomes

$$\frac{1}{c^2}\frac{\partial^2\mathbf{A}}{\partial t^2} = \frac{\partial^2\mathbf{A}}{\partial x^2}.$$

Now, we shall use the 4-vector notation

$$\mathsf{x} \equiv (t, \mathbf{x}), \quad \mathsf{k} \equiv (\omega, \mathbf{k}),$$

so that their scalar product is

$$\mathsf{k} \cdot \mathsf{x} = \omega t - \mathbf{k} \cdot \mathbf{x}.$$

Hence, plane waves are written as

$$\mathbf{A} = \mathbf{A}_0 e^{i\mathsf{k}\cdot\mathsf{x}}.$$

So, computing the two halfs of the wave equation,

$$\begin{aligned} \frac{\partial^2 \mathbf{A}}{\partial t^2} &= -\omega^2 \mathbf{A}, \\ \frac{\partial^2 \mathbf{A}}{\partial x^2} &= -|\mathbf{k}|^2 \mathbf{A}. \end{aligned}$$

Hence, the wave equation requires that

$$\frac{\omega^2}{c^2} = |\mathbf{k}|^2,$$

which is the standard dispersion relation

$$\omega = c|\mathbf{k}|.$$

Now, the most general solution to the wave equation is a sum over modes. Infact, in addition to summing over modes, we must also sum over polarisation states. So, the most general solution is

$$\mathbf{A}(\mathsf{x}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \sum_{\lambda=1,2} \left(\boldsymbol{\varepsilon}_{\mathbf{k},\lambda} a_{\mathbf{k},\lambda} e^{-i\mathsf{k}\cdot\mathsf{x}} + \boldsymbol{\varepsilon}^*_{\mathbf{k},\lambda} a^\dagger_{\mathbf{k},\lambda} e^{i\mathsf{k}\cdot\mathsf{x}} \right). \tag{8.8}$$

To compound the point, the coefficient-vector $\boldsymbol{\varepsilon}_{\mathbf{k},\lambda}$ is a polarisation coefficient (where there are λ polarisations), and $a_{\mathbf{k},\lambda}$ is some amplitude. Both coefficients may be complex, and are classical in nature. The factor of V is some volume-normalisation. We require that

$$\mathbf{k} \cdot \boldsymbol{\varepsilon}_{\mathbf{k},\lambda} = 0,$$

due to the transverse nature that arises from use of the Coulomb gauge.

The classical value of the energy of the electromagnetic field is given by

$$H_{EM} = \frac{1}{8\pi} \int (\mathbf{E}^2 + \mathbf{B}^2) d\mathbf{x}.$$

Now, we have that in free space,

$$\mathbf{E}^2 = \frac{\omega^2}{c^2} \mathbf{A}^2.$$

So, we can compute that

$$\frac{1}{8\pi} \int \mathbf{E}^2 dx = \frac{1}{4\pi} \sum_{\mathbf{k},\lambda} \frac{\omega^2}{c^2} a^\dagger_{\mathbf{k},\lambda} a_{\mathbf{k},\lambda} = \frac{1}{8\pi} \int \mathbf{B}^2 dx,$$

and hence that

$$H_{EM} = \frac{1}{2\pi} \sum_{\mathbf{k},\lambda} \frac{\omega^2}{c^2} a^\dagger_{\mathbf{k},\lambda} a_{\mathbf{k},\lambda}.$$

Now, if we introduce

$$\begin{aligned} Q_{\mathbf{k},\lambda} &= \frac{2\sqrt{\pi}}{c} \left(a_{\mathbf{k},\lambda} + a^\dagger_{\mathbf{k},\lambda} \right), \\ P_{\mathbf{k},\lambda} &= -\frac{2\sqrt{\pi}}{c} i\omega \left(a_{\mathbf{k},\lambda} - a^\dagger_{\mathbf{k},\lambda} \right), \end{aligned}$$

we find that the Hamiltonian can be written as

$$H_{EM} = \frac{1}{2} \sum_{\mathbf{k},\lambda} \left(P^2_{\mathbf{k},\lambda} + \omega^2 Q^2_{\mathbf{k},\lambda} \right).$$

This is of the same form as the harmonic oscillator. That is, in expanding the general solution into its modes, we have found that the Hamiltonian of the electromagnetic radiation is the same as a sum over modes of the harmonic oscillators. That is, we can think of radiation as being lots of little harmonic oscillators.

So, let us "quantise the theory", by sending quantities to operators:

$$P_{\mathbf{k},\lambda} \longmapsto \hat{P}_{\mathbf{k},\lambda}, \quad Q_{\mathbf{k},\lambda} \longmapsto \hat{Q}_{\mathbf{k},\lambda}.$$

Also, we notice that the above definitions allow us to compute the commutators,

$$\begin{aligned} \left[\hat{P}_{\mathbf{k},\lambda}, \hat{Q}_{\mathbf{k}',\lambda'} \right] &= i\hbar \delta_{\mathbf{k}\mathbf{k}'} \delta_{\lambda\lambda'}, \\ \left[\hat{P}_{\mathbf{k},\lambda}, \hat{P}_{\mathbf{k}',\lambda'} \right] &= 0, \\ \left[\hat{Q}_{\mathbf{k},\lambda}, \hat{Q}_{\mathbf{k}',\lambda'} \right] &= 0. \end{aligned}$$

We redefine the *creation and annihilation* operators,

$$\hat{a}_{\mathbf{k},\lambda} = \frac{1}{\sqrt{2\hbar\omega}} \left(\omega \hat{Q}_{\mathbf{k},\lambda} + i \hat{P}_{\mathbf{k},\lambda} \right), \tag{8.9}$$

$$\hat{a}^\dagger_{\mathbf{k},\lambda} = \frac{1}{\sqrt{2\hbar\omega}} \left(\omega \hat{Q}_{\mathbf{k},\lambda} - i \hat{P}_{\mathbf{k},\lambda} \right), \tag{8.10}$$

where we see that the commutator holds,

$$\left[\hat{a}_{\mathbf{k},\lambda}, \hat{a}^\dagger_{\mathbf{k}',\lambda'} \right] = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\lambda\lambda'}, \tag{8.11}$$

with all others being zero. Hence, we see that we can write the Hamiltonian as

$$\hat{\mathcal{H}}_{EM} = \sum_{\mathbf{k},\lambda} \hbar\omega \left(\hat{a}^\dagger_{\mathbf{k},\lambda} \hat{a}_{\mathbf{k},\lambda} + \frac{1}{2} \right). \tag{8.12}$$

This gives us an example of quantising a field. We take a field, we expand the solution in terms of modes of the field, where each mode is just a harmonic oscillator. We then apply the quantisation scheme to each oscillator, writing commutation relations.

We write the eigenstates as

$$|N_{EM}\rangle = |n_{\mathbf{k}_1,\lambda_1}, n_{\mathbf{k}_2,\lambda_2}, \ldots\rangle = |n_{\mathbf{k}_1,\lambda_1}\rangle |n_{\mathbf{k}_2,\lambda_2}\rangle \ldots,$$

where $n_{\mathbf{k}_i,\lambda_j}$ is the occupancy number of a particular state. That is, how many photons with a given wavenumber and polarisation state.

We write the eigenvalues as

$$E_{EM} = \sum_{\mathbf{k},\lambda} \hbar\omega_{\mathbf{k},\lambda} \left(n_{\mathbf{k},\lambda} + \frac{1}{2} \right).$$

Now, if one recalls that

$$\frac{d}{dt}\hat{Q}(t) = -\frac{i}{\hbar}\left[\hat{Q}, \hat{\mathcal{H}}\right],$$

then we see that we can find the Heisenberg operator. That is, use the non-time dependent operator to construct the time dependent operator. Now,

$$\frac{d}{dt}\hat{a}_{\mathbf{k}',\lambda'}(t) = -\frac{i}{\hbar}\left[\hat{a}_{\mathbf{k}',\lambda'}, \hat{\mathcal{H}}\right].$$

For notational brevity, we shall now leave off the λ subscript. So, the commutator is

$$\begin{aligned}\left[\hat{a}_{\mathbf{k}'}, \hat{\mathcal{H}}\right] &= \hat{a}_{\mathbf{k}'}\hat{\mathcal{H}} - \hat{\mathcal{H}}\hat{a}_{\mathbf{k}'} \\ &= \sum_{\mathbf{k}} \hbar\omega \left(\hat{a}_{\mathbf{k}'}\hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}} - \hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}}\hat{a}_{\mathbf{k}'} \right).\end{aligned}$$

Now, by our commutation relations, we can swap the order of the very last two terms, to give

$$\left[\hat{a}_{\mathbf{k}'}, \hat{\mathcal{H}}\right] = \sum_{\mathbf{k}} \hbar\omega \left(\hat{a}_{\mathbf{k}'}\hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}} - \hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}'}\hat{a}_{\mathbf{k}} \right),$$

which we then write as

$$\left[\hat{a}_{\mathbf{k}'}, \hat{\mathcal{H}}\right] = \sum_{\mathbf{k}} \hbar\omega \left(\left[\hat{a}_{\mathbf{k}'}, \hat{a}^\dagger_{\mathbf{k}}\right] \hat{a}_{\mathbf{k}} \right).$$

Hence, using our commutation relation, this is just

$$\begin{aligned}\left[\hat{a}_{\mathbf{k}'}, \hat{\mathcal{H}}\right] &= \sum_{\mathbf{k}} \hbar\omega\delta_{\mathbf{k}'\mathbf{k}}\hat{a}_{\mathbf{k}} \\ &= \hbar\omega\hat{a}_{\mathbf{k}'}.\end{aligned}$$

Therefore, we see that

$$\begin{aligned}\frac{d}{dt}\hat{a}_{\mathbf{k}}(t) &= -\frac{i}{\hbar}\left[\hat{a}_{\mathbf{k}}, \hat{\mathcal{H}}\right] \\ &= -i\omega\hat{a}_{\mathbf{k}}.\end{aligned}$$

This is easily integrated, to give

$$\hat{a}_{\mathbf{k},\lambda}(t) = e^{-i\omega t}\hat{a}_{\mathbf{k},\lambda}(0). \tag{8.13}$$

In a similar way, we can show that

$$\hat{a}^{\dagger}_{\mathbf{k},\lambda}(t) = e^{i\omega t}\hat{a}^{\dagger}_{\mathbf{k},\lambda}(0). \tag{8.14}$$

Therefore, we have expressions for the time dependent creation and annihilation operators.

The action of the creation operator:

$$\hat{a}^{\dagger}_{\mathbf{k}',\lambda'}|N_{EM}\rangle = \sqrt{n_{\mathbf{k}',\lambda'}+1}|n_{\mathbf{k}_1,\lambda_1},\ldots,n_{\mathbf{k}',\lambda'}+1,\ldots\rangle. \tag{8.15}$$

The action of the destruction operator:

$$\hat{a}_{\mathbf{k}',\lambda'}|N_{EM}\rangle = \sqrt{n_{\mathbf{k}',\lambda'}}|n_{\mathbf{k}_1,\lambda_1},\ldots,n_{\mathbf{k}',\lambda'}-1,\ldots\rangle. \tag{8.16}$$

We can now write the field operator,

$$\hat{\mathbf{A}}(\mathbf{x},t) = c\sqrt{\frac{2\pi\hbar}{\omega V}}\sum_{\mathbf{k},\lambda}\left(e^{-i\mathbf{k}\cdot\mathbf{x}}\boldsymbol{\varepsilon}_{\mathbf{k},\lambda}\hat{a}_{\mathbf{k},\lambda}(0) + e^{i\mathbf{k}\cdot\mathbf{x}}\boldsymbol{\varepsilon}^{*}_{\mathbf{k},\lambda}\hat{a}^{\dagger}_{\mathbf{k},\lambda}(0)\right),$$

where the first term "kills" a wave, and the second term "creates" a wave. Notice that by (8.13) and (8.14), we can rewrite this operator in terms of the time dependent creation/destruction operators, being careful of expressions like

$$e^{i\mathbf{k}\cdot\mathbf{x}}\hat{a}(0) = e^{i\omega t + i\mathbf{x}\cdot\mathbf{k}}\hat{a}(0) = e^{i\mathbf{k}\cdot\mathbf{x}}\hat{a}(t).$$

Hence, the field operator:

$$\hat{\mathbf{A}}(\mathbf{x},t) = c\sqrt{\frac{2\pi\hbar}{\omega V}}\sum_{\mathbf{k},\lambda}\left(e^{i\mathbf{k}\cdot\mathbf{x}}\boldsymbol{\varepsilon}_{\mathbf{k},\lambda}\hat{a}_{\mathbf{k},\lambda}(t) + e^{-i\mathbf{k}\cdot\mathbf{x}}\boldsymbol{\varepsilon}^{*}_{\mathbf{k},\lambda}\hat{a}^{\dagger}_{\mathbf{k},\lambda}(t)\right). \tag{8.17}$$

Thus, again, we see that the first term destroys a photon in state $(\mathbf{k},\lambda)$ and the second term destroys a photon in the state $(\mathbf{k},\lambda)$.

Issues Now, if one recalls the Coulomb gauge $\nabla\cdot\mathbf{A} = 0$, one must question the meaning of $\nabla\cdot\hat{\mathbf{A}} = 0$; the equivalent in the quantised field operator formalism. The interesting thing is that there is no real consensus as it its meaning!

Another interesting point, is the "plane wave" assumption: we expanded the modes in terms of plane waves. This seems sensible enough, if the space is "empty enough". That is, there are no walls anywhere near our system. In most circumstances, this is ok, and experiment agrees. However, if one does an experiment based in a small cavity, then plane waves are not a good thing to expand in terms of. Indeed, experiments based in small cavities find different transition probabilities to those in "open space".

8.3.1 Zero Point Energy

Recall that the eigenvalues (i.e. energy of a particular state) are written as

$$E_{EM} = \sum_{\mathbf{k},\lambda} \hbar\omega_{\mathbf{k},\lambda} \left(n_{\mathbf{k},\lambda} + \frac{1}{2} \right),$$

where $n_{\mathbf{k},\lambda}$ is the number of photons in a given state. Suppose that there are no photons at all in a system. Then, there is a non-zero energy of

$$E_{ZP} = \sum_{\mathbf{k},\lambda} \frac{1}{2} \hbar\omega_{\mathbf{k},\lambda}.$$

This energy is known as the *zero-point energy*. We can crudely compute this value. Consider sending the sum to an integral,

$$\sum_{k,\lambda} \longmapsto 2 \int_0^{k_{max}} \frac{k^2}{(2\pi)^3} dk,$$

where we have used a factor of 2 due to the two polarisation states. If we then use the dispersion relation $\omega = ck$, the zero-point energy is just

$$E_{ZP} = \int_0^{k_{max}} \frac{\hbar c k^3}{(2\pi)^3} dk = \frac{\hbar c}{32\pi^3} k_{max}^4.$$

Now, there is no "real limit" to the maximum wavenumber k_{max}, hence, an infinite zero-point energy!

To get a handle on how much energy this is, consider an example where we impose that the maximum wavenumber is that of blue light. Then, $\lambda_{blue} \approx 4$nm, with

$$k_{max} = \frac{2\pi}{\lambda} \quad \Rightarrow \quad E_{ZP} = \frac{\hbar c \pi}{2\lambda_{max}^4} \approx 1.8 Jm^{-3}.$$

The energy of a typical lamp is $\approx 2.7 \times 10^{-8} Jm^{-3}$.

For fermions, the Hamiltonian is

$$\hat{\mathcal{H}} = \sum_{\mathbf{k},\lambda} \hbar\omega_{\mathbf{k},\lambda} \left(\hat{a}^\dagger_{\mathbf{k},\lambda} \hat{a}_{\mathbf{k},\lambda} - \frac{1}{2} \right).$$

So, notice that upon adding this to the Hamiltonian for radiation (as above), the Hamiltonians cancel, leaving no zero-point energy. This is the general idea in SUperSymmetrY (SUSY), whereby each boson has an accompanying fermion (and vice-versa), which ends up canceling out the zero-point energy.

Casimir Effect There is an experiment which can test for the validity of the plane-wave expansion, and the zero-point energy. Consider putting two parallel mirrors a distance L apart. Then, along the axis the plane wave expansion will be ok, and radiation will act as a load of harmonic oscillators. Along the axis perpendicular to the mirrors, the waves will have to be discrete, in terms of $k_x = 2\pi n/L$ where $n = 1, 2, 3, \ldots$. So now, upon computing the zero-point energy, we can turn the sum into an integral for the k_y and k_z modes, but not the k_x modes (as they are not continuous). Hence, the zero-point energy is computed via

$$E_{ZP} = \sum_{k_x} \int\int c(k_x^2 + k_y^2 + k_z^2)^{1/2} \frac{dk_y dk_z}{(2\pi)^2} \sim \frac{1}{L^3}.$$

Now, the force is just

$$F = \frac{\partial E_{ZP}}{\partial L} = -\frac{\hbar c \pi^2}{240 L^4}.$$

That there is a negative force means that there is an attraction between the two plates. Therefore, we see that if this zero-point energy is to exist, then there should be a force between two plates in "vacuum". Indeed, experiment confirms this.

8.3.2 Coherence & Radiation

The states of the EM field are $|N\rangle$, whereby

$$\langle N|\hat{E}|N\rangle = 0.$$

Now, there is the usual uncertainty relation between the state and phase of the EM field,

$$\Delta N \Delta\varphi \geq 1.$$

Now, states produces by the creation/annihilation operators are coherent,

$$\hat{a}|z\rangle = z|z\rangle,$$

and in this case

$$\Delta N \Delta\varphi = 1.$$

Transition probabilities are given by the matrix elements

$$-\frac{e}{mc}\langle N'|\hat{\mathbf{A}} \cdot \hat{\mathbf{p}}|N\rangle,$$

where we have that the field operator is of the form

$$\hat{\mathbf{A}} \sim \alpha\hat{a} + \beta\hat{a}^\dagger.$$

Hence, as the action of the creation operator, upon a state with $n_{\mathbf{k},\lambda}$ will send that state to one with $n_{\mathbf{k},\lambda}+1$, and the annihilation operator to a state $n_{\mathbf{k},\lambda}-1$. Therefore, we are sending the initial state $|N\rangle$ to some other state.

$$|N\rangle = |N_a, n_{\mathbf{k}\lambda}\rangle \to |N_a, n_{\mathbf{k}\lambda} \pm 1\rangle.$$

Hence, by orthonormality of the $|N\rangle$ states, we must have that $\langle N'| = |N_a, n_{\mathbf{k}\lambda} \pm 1\rangle$. Hence,

- If $|N'\rangle = |N_a, n_{\mathbf{k}\lambda} + 1\rangle$, then there is creation of a photon,
- If $|N'\rangle = |N'_a, n_{\mathbf{k}\lambda} - 1\rangle$, then there is absorption of a photon.

Hence, the matrix element for absorption is

$$V^{abs}_{N'N} = -\frac{e}{mc} c \sqrt{\frac{2\pi\hbar}{\omega V}} \langle N'_a, n_{\mathbf{k},\lambda} - 1 | e^{i\mathbf{k}\cdot\mathbf{x}} \hat{a}_{\mathbf{k},\lambda}(t) \hat{\mathbf{p}} \boldsymbol{\varepsilon}_{\mathbf{k},\lambda} | N_a, n_{\mathbf{k},\lambda} \rangle,$$

where we have used that the field operator collapses down to just the creation operator. Hence, we write this as

$$V^{abs}_{N'N} = -\frac{e}{m} \sqrt{\frac{n_{\mathbf{k},\lambda} 2\pi\hbar}{\omega V}} \langle N'_a | e^{i\mathbf{k}\cdot\mathbf{x}} \hat{\mathbf{p}} \boldsymbol{\varepsilon}_{\mathbf{k},\lambda} | N_a \rangle e^{-i\omega t}.$$

If we use the dipole approximation, which is $e^{i\mathbf{k}\cdot\mathbf{x}}$=1, the matrix element goes to

$$\langle N'_a | \hat{\mathbf{p}} \boldsymbol{\varepsilon}_{\mathbf{k},\lambda} | N_a \rangle = im \frac{E_{N_a} - E_{N'_a}}{\hbar c} \mathbf{d}_{N'N} \boldsymbol{\varepsilon}_{\mathbf{k},\lambda}.$$

Basically, one can see that

$$\left| V^{abs}_{N'N} \right|^2 \propto n_{\mathbf{k},\lambda},$$

and from a similar line of argument,

$$\left| V^{emis}_{N'N} \right|^2 \propto n_{\mathbf{k},\lambda} + 1.$$

In this emission matrix element, the $n_{\mathbf{k},\lambda}$-part is due to stimulation, and the +1-part due to spontaneous emission.