Notes on Quantum Mechanics: Bound States

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1 Energy Eigenstates

As a postulate of QM, we have the Schrödinger Equation:

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle \tag{1}$$

where $|\psi\rangle$ is a wave function, and $\hat{H} = \frac{\hat{P}^2}{2m} + V(\hat{X})$ is the quantum Hamiltonian operator. It is understood that $\hat{P}$ and $\hat{X}$ are OPERATORS, and thus they are **represented by different matrices in different vector bases**. That is, in different bases, $\hat{P}$ and $\hat{X}$ will have different actions upon vectors in that space. I will drop the hat notation for visual ease.

To solve this equation, we turn it into an eigenvalue problem by considering the eigenkets of H:

$$H|E\rangle = E|E\rangle$$

Such kets labeled by E are called **Energy Eigenstates**. We can then write $|\psi(t)\rangle$ in terms of $|E\rangle$

$$|\psi(t)\rangle = I|\psi(t)\rangle = \sum_E |E\rangle\langle E|\psi(t)\rangle \equiv \sum_E a_E(t)|E\rangle$$

Since H is a linear operator:

$$\begin{aligned} H|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle &= \sum_E i\hbar\frac{\partial}{\partial t}a_E(t)|E\rangle \\ &= \sum_E a_E(t)H|E\rangle = \sum_E a_E(t)E|E\rangle \end{aligned}$$

to clean it up

$$\sum_E i\hbar\frac{\partial}{\partial t}a_E(t)|E\rangle = \sum_E a_E(t)E|E\rangle$$

so

$$i\hbar\frac{\partial}{\partial t}a_E(t) = a_E(t)E$$

this is an easy equation to solve:

$$\frac{\partial}{\partial t}a_E(t) = -\frac{iE}{\hbar}a_E(t) \Rightarrow \boxed{a_E(t) = a_E(0)e^{-\frac{iEt}{\hbar}}} \tag{2}$$

Having obtained the components of $|\psi\rangle$ when expanded in the $|E\rangle$ basis, we get $|\psi\rangle$ as follows:

$$\boxed{|\psi\rangle = \sum_E a_E(0)e^{-\frac{iEt}{\hbar}}|E\rangle} \tag{3}$$

This is a useful result: **Energy Eigenstates evolve by a simple phase, and therefore any observable values associated with them have preserved probabilities and thus expectation values**. For this reason, energy eigenstates are also called **stationary states**. we can also write $|\psi\rangle$ in terms of $|\psi\rangle$'s initial state as follows:

$$|\psi(t)\rangle = \sum_E \langle E|\psi(0)\rangle e^{-\frac{iEt}{\hbar}}|E\rangle = \sum_E |E\rangle\langle E|\psi(0)\rangle e^{-\frac{iEt}{\hbar}} = \sum_E \left(|E\rangle\langle E|e^{-\frac{iEt}{\hbar}}\right)|\psi(0)\rangle \tag{4}$$

we introduce the following definition:

$$U_E(t) \equiv \left(|E\rangle\langle E|e^{-\frac{iEt}{\hbar}}\right)$$
$$U(t) \equiv \sum_E U_E(t)$$

so that

$$|\psi(t)\rangle = \left(\sum_E U_E(t)\right)|\psi(0)\rangle = U(t)|\psi(0)\rangle$$

If the eigenspace for $|E\rangle$ is degenerate, we can also introduce an extra label to specify the different eigenkets for the same eigenvalue:

$$U(t) = \sum_E \left(\sum_\gamma |E,\gamma\rangle\langle E,\gamma|\right) e^{-\frac{iEt}{\hbar}}$$

$U(t)$ is called the **propagator**. In case that the space of eigenvalues is continuous, we need to replace the discrete sum with an integral. Therefore, our general strategy when solving the Schrödinger Equation is to find the energy eigenstates of the Hamiltonian in the given system, construct the propagator from them and attach it to the initial state of the system; that completely determines the state of the system for all future times t. Below are some examples of this process.

2 The Free Particle

The Free Particle system has the Hamiltonian operator $H = \frac{P}{2m} + 0$; i.e. $V(X) = 0$:

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle = \frac{P^2}{2m}|\psi\rangle$$

This problem can be solved without going into any basis, but I personally prefer going into one. In the X basis, $P = -i\hbar\frac{\partial}{\partial x}$. Let us find the energy eigenfunctions:

$$E|E\rangle = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}|E\rangle$$

rearranging gives

$$-\frac{2mE}{\hbar^2}|E\rangle = \frac{d^2}{dx^2}|E\rangle$$

this is a fairly easy equation to solve:

$$|E,+k\rangle = e^{ikx},\ |E,-k\rangle = e^{-ikx}$$
$$k \equiv \sqrt{\frac{2mE}{\hbar^2}}$$

Therefore, the eigenspace for each eigenenergy value is twofold-degenerate. One for $+k$ and one for $-k$. Having found the energy eigenstates, let us express the general solution to this problem in the spirit of Eqaution (3):

$$|\psi\rangle = \int_0^\infty \sum_{\gamma(E)\in\{+k(E),-k(E)\}} c_\gamma e^{-\frac{iEt}{\hbar}}|E,\gamma(E)\rangle\, dE$$

There is a notable result here: eigenkets of H are also eigenkets of P for a free particle. Therefore, we can expand the state of a free particle in terms of its momentum eigenkets as well, and they would still **evolve by a simple phase**. Since eigenspaces of E are degenerate, we can talk in terms of k instead. In the k representation, the general solution is as follows:

$$\langle x|\psi\rangle \equiv |\psi(x,t)\rangle = \int_{-\infty}^{\infty} c(k)\langle x|k\rangle e^{-i\frac{\hbar k^2}{2m}t}\, dk = \int_{-\infty}^{\infty} c(k)e^{ikx}e^{-i\frac{\hbar k^2}{2m}t}\, dk \tag{5}$$

Note that we let k run from $-\infty$ to ∞ in the integral because it is continuous and can run negative, unlike energy. Oftentimes, a normalization constant of $\frac{1}{\sqrt{2\pi}}$ is extracted out of the $c(k)$ for convenience, as one often would have to work with Gaussian wave packets. The coefficients $c(k)$ can be found via orthogonality

$$c(k) = \langle k|\psi\rangle = \int_{-\infty}^{\infty} \langle k|x\rangle\langle x|\psi\rangle\, dx = \int_{-\infty}^{\infty} \langle x|k\rangle^*\langle x|\psi\rangle\, dx = \int_{-\infty}^{\infty} e^{-ikx}\psi(x)\, dx$$

We can construct the propagator as follows:

$$U(t) = \int_{-\infty}^{\infty} |k\rangle\langle k|e^{-\frac{iE(k)t}{\hbar}}\, dk = \int_{-\infty}^{\infty} |k\rangle\langle k|e^{-i\frac{\hbar k^2}{2m}t}\, dk$$

There is something important to note: energy eigenstates by themselves are **not** normalizable. It is only when we superimpose them into a wave packet do they become physical models of particles.

3 Infinite Square Well

The infinite square well Hamiltonian is given by $H = \frac{P^2}{2m} + V(X)$, where

$$V(x) = \begin{cases} \infty & |x| > \frac{a}{2} \\ 0 & |x| \leq \frac{a}{2} \end{cases}$$

where a is the width of the "well" that traps a system. The system is identical to the free particle when considering only inside the well, that is, the general energy eigenfunction in the X basis is

$$|\psi(x)\rangle = Ae^{ikx} + Be^{-ikx}, \quad k \equiv \sqrt{\frac{2mE}{\hbar^2}}$$

if we went through the same process as we did for the free particle. However, different from the free particle, the infinite square well particle is constrained by the well such that

$$|\psi(x = -\frac{L}{2})\rangle = Ae^{-\frac{ikL}{2}} + Be^{\frac{ikL}{2}} = 0$$
$$|\psi(x = \frac{L}{2})\rangle = Ae^{\frac{ikL}{2}} + Be^{-\frac{ikL}{2}} = 0$$

Combining and rearranging these two equations gives us $1 - e^{2ikL} = 0$, then

$$e^{2ikL} = (e^{ikL})^2 = 1$$

so

$$e^{ikL} = \pm 1$$

this constraints kL:

$$kL = n\pi, \quad n = 0, \pm 1, \pm 2, ...$$

With this knowledge, we can also fix the ratio of A and B with either of the equations:

$$A + Be^{ikL} = A + Be^{in\pi} = A + (-1)^n B = 0$$
$$A = (-1)^{n+1}B$$

for even n we have:

$$\begin{aligned} |\psi_{even}(x)\rangle &= A(\cos(kx) + i\sin(kx)) + B(\cos(-kx) + i\sin(-kx)) \\ &= A(\cos(kx) + i\sin(kx)) - A(\cos(kx) - i\sin(kx)) \\ &= 2Ai\sin(kx) \end{aligned}$$

The i in the wave function is simply a phase $i = e^{i\frac{\pi}{2}}$, which can be acquired through time evolution if the system started out in a purely real wave function. It is therefore not intrinsic to the infinite

square well system since the system can acquire any arbitrary phase via time evolution — we disregard it. For odd n we have:

$$\begin{aligned}|\psi_{odd}(x)\rangle &= A(\cos(kx) + i\sin(kx)) + B(\cos(-kx) + i\sin(-kx)) \\ &= A(\cos(kx) + i\sin(kx)) + A(\cos(kx) - i\sin(kx)) \\ &= 2A\cos(kx)\end{aligned}$$

By the requirement of normalization

$$A = \frac{1}{\sqrt{2L}}$$

and therefore we have the following solutions for the infinite square well:

$$|\psi_{even}(x)\rangle = \sqrt{\frac{2}{L}}\sin(\frac{n\pi}{L}x)$$
$$|\psi_{odd}(x)\rangle = \sqrt{\frac{2}{L}}\cos(\frac{n\pi}{L}x)$$

This is an interesting result — only **discrete** energy levels are admissible in the infinite square well. In addition, the state for which $n = 0$ is aphysical and is of little interest since $|\psi\rangle = 0$; the particle does not even exist! Given these energy eigenfunctions, any particle in a box can be modeled by an arbitrary superposition of them, and they would all evolve with a simple phase. The propagator for this system will not be discussed.

A system like the particle in a box where the energy of the states are strictly bound by the potential on both sides is said to be **bound**, in contrast to the free particle, where continuous energy levels are allowed. Generally, it can be shown that a bound state will *always* have discrete energy levels while free states will have continuous energy levels. This fact can be mathematically argued using the fact that the solution to the Schrödinger Equation is *exponentially* increasing/decreasing when the particle is in a classically disallowed region ($V < E$). Without going into too much mathematics, say that we wanted to "tune" the derivative of the wave function such that the exponentially growing term is eliminated on one side, it is generally not the case that the other side will be dampened as well. Only for certain energy values, it is possible to eliminate the growing exponentials on both sides of a bounding potential — these are our discrete energy levels.

4 Aside: Wave functions in Position and Momentum Space

To evaluate a certain wave function in some basis, we take the inner product of a basis ket with the ket that represents the wave function. To evaluate a wave function in the X (position) and K (momentum ignoring a factor of $\hbar$) bases respectively, we have:

$$\langle x|\psi\rangle \equiv \psi_x(x)$$
$$\langle k|\psi\rangle \equiv \psi_k(k)$$

We can rewrite them as follows:

$$\psi_x(x) = \langle x|\psi\rangle = \int \langle x|k\rangle\langle k|\psi\rangle\, dk = \int \langle x|k\rangle\psi_k(k)\, dk$$
$$\psi_k(k) = \langle k|\psi\rangle = \int \langle k|x\rangle\langle x|\psi\rangle\, dx = \int \langle x|k\rangle^*\psi_x(x)\, dx$$

We now need to find $|k\rangle$ evaluated in the X basis. That is not terribly hard; a quick argument will show that

$$\langle x|k\rangle = Ae^{ikx} \tag{6}$$

The argument is as follows. Since in the X basis, K's action is the following:

$$K = -i\frac{\partial}{\partial x}$$

We can now look at eigenkets of K:

$$K|k\rangle = k|k\rangle$$

This eigenvalue problem turns into an easy differential equation to solve in the X basis:

$$-i\frac{\partial}{\partial x}\langle x|k\rangle = k\langle x|k\rangle$$

Solving this equation would yield Equation (6). The constant A is chosen to be $\frac{1}{\sqrt{2\pi}}$ so that momentum eigenkets normalize to the Dirac Delta function:

$$\langle k|k'\rangle = \int_{-\infty}^{\infty}\langle k|x\rangle\langle x|k'\rangle\,dx = \frac{1}{2\pi}\int_{-\infty}^{\infty}e^{i(k'-k)x}\,dx = \delta(k'-k)$$

The expectation value of position in the X basis is simply given by

$$\langle X\rangle = \langle\psi_x|X|\psi_x\rangle = \int_{-\infty}^{\infty}\psi^*(x)x\psi(x)\,dx = \int_{-\infty}^{\infty}|\psi(x)|^2x\,dx$$

but the expectation value of momentum is much more complicated

$$\langle P\rangle = \langle\psi_x|\hbar K|\psi_x\rangle = \int_{-\infty}^{\infty}\psi_x^*(x)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi(x)\,dx$$

however, in the K basis, this calculation has a simple answer

$$\langle P\rangle = \langle\psi_k|\hbar K|\psi_k\rangle = \int_{-\infty}^{\infty}\psi_k^*(k)\hbar k\psi_k(k)\,dk = \int_{-\infty}^{\infty}|\psi_k(k)|^2\hbar k\,dk$$

As we have seen, the relationship between ψ_k and ψ_x is that of a Fourier Transform, and this relationship provides an alternative way to evaluate the expectation values of momentum in the X basis rather than by brute-force differentiation under the integral.

More generally, it can be shown that

$$\langle f(P)\rangle = \langle\psi_k|f(P)|\psi_k\rangle = \int_{-\infty}^{\infty}|\psi_k(k)|^2f(\hbar k)\,dk$$

The proof is as follows. We start out by expanding $f(P)$ with Taylor Series:

$$\begin{aligned}\langle f(P)\rangle &= \left\langle f(0) + Pf'(0) + P^2\frac{f''(0)}{2!} + P^3\frac{f'''(0)}{3!} + ...\right\rangle \\ &= \langle f(0)\rangle + \langle Pf'(0)\rangle + \left\langle\frac{f''(0)}{2!}\right\rangle + \left\langle P^3\frac{f'''(0)}{3!}\right\rangle + ... \\ &= f(0) + \langle P\rangle f'(0) + \left\langle P^2\right\rangle\frac{f''(0)}{2!} + \left\langle P^3\right\rangle\frac{f'''(0)}{3!} + ...\end{aligned}$$

we then evaluate the expectation values of P in the K basis:

$$\begin{aligned}\langle f(P)\rangle &= f(0) + \langle\psi_k|P|\psi_k\rangle f'(0) + \left\langle\psi_k|P^2|\psi_k\right\rangle\frac{f''(0)}{2!} + \left\langle\psi_k|P^3|\psi_k\right\rangle\frac{f'''(0)}{3!} + \dots \\ &= f(0) + \int_{-\infty}^{\infty}|\psi_k(k)|^2\hbar k\,dk\,\frac{f'(0)}{2!} + \int_{-\infty}^{\infty}|\psi_k(k)|^2(\hbar k)^2\,dk\,\frac{f''(0)}{2!} + \dots \\ &= \int_{-\infty}^{\infty}|\psi_k(k)|^2\left(f(0) + \hbar kf'(0) + (\hbar k)^2\frac{f''(0)}{2!} + \dots\right)dk \\ &= \int_{-\infty}^{\infty}|\psi_k(k)|^2f(\hbar k)\,dk\end{aligned}$$

where $\hbar k$ is the action of P in the K basis.

The relationship between position and momentum space hints at the important Uncertainty Principle that permeates QM. Here is a stab at it. Consider a very localized wave function in position space:

$$\psi_x(x) = \delta(x)$$

the expectation value of position is trivially 0 in this case. However, when we go into momentum space, the story is a lot more different:

$$\psi_k(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \delta(x)\, dx = \frac{1}{\sqrt{2\pi}}$$

$\psi_k(k)$ yields a *uniform* probability distribution — that is, it is fair game to find the momentum of the particle at *any* momentum eigenvalue. Therefore the uncertainty in momentum is very large compared to the uncertainty in position. Let us then consider a wave function that has low uncertainty in momentum:

$$\psi_x(x) = e^{ikx}$$

the expectation value of momentum is trivially $\hbar k$ in this case. We can easily show this with a Fourier Transform:

$$\psi_k(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ik'x} e^{ikx}\, dx = \delta(k - k')$$

However, the uncertainty in position is huge compared to that of momentum as e^{ikx} is a plane wave that extends undiminished into infinity.

In general, the more certain about position we are, the less certain about momentum we *can be*, no matter how accurate our measurements can be. A famous thought experiment by Heisenberg (see Heisenberg's Microscope) used the argument that if we use light to measure the position of some particle, then upon knowing the position of the particle, the light would have also imparted some energy and thus momentum to the particle — thus introducing uncertainty. The smaller the wavelength the light, the more certain we can be about the position, but also the greater the energy imparted to the particle. This is the basis of the **Heisenberg Uncertainty Principle** that we shall explore later.

5 Dirac Well

The Dirac well Hamiltonian is given by $H = \frac{P^2}{2m} - \alpha V_o \delta(x)$. We only consider bound states here, so we would work with a E such that $E < V_o$. We first solve the Schrödinger Equation for $x < 0$, or equivalently $V(x) = 0$:

$$\frac{P^2}{2m}|E\rangle = E|E\rangle$$

rearranging and going into the X basis gives

$$\frac{\partial^2}{\partial x^2}\langle x|E\rangle = -\frac{2mE}{\hbar^2}\langle x|E\rangle \equiv \kappa^2 \langle x|E\rangle$$

where

$$\kappa \equiv \sqrt{\frac{-2mE}{\hbar^2}} \in \mathbb{R}$$

The general solution to this equation is

$$\langle x|E\rangle \equiv \psi_E(x) = Ae^{\kappa x} + Be^{-\kappa x}$$

the second term blows up as $x \to -\infty$, and thus $B = 0$. The same logic can be applied to $x > 0$ such that we have the following two wave functions for left and right respectively:

$$\psi_L(x) = Ae^{\kappa x}$$
$$\psi_R(x) = Fe^{-\kappa x}$$

We require the wave function to be continuous at $x = 0$, so $A = F$. The derivative of the wave function however, is not continuous at $x = 0$ as e^x and e^{-x} forms a cusp at $x = 0$. We can still, however, work with the derivatives:

$$\psi_L'(x) = \kappa A e^{\kappa x}$$
$$\psi_R'(x) = -\kappa A e^{-\kappa x}$$

The change in the derivative at $x = 0$ is then

$$\Delta \equiv -2\kappa A$$

The change in derivative can also be computed as follows:

$$\Delta = \int_{0-\epsilon}^{0+\epsilon} \left(\frac{d^2\psi}{dx^2} \right) dx$$

where ϵ is an infinitesimal number. By the Schrödinger Equation:

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2} \left(E + \alpha V_o \delta(x) \right) \psi$$

so we can evaluate the integral as follows:

$$\begin{aligned} -\frac{2m}{\hbar^2} \int_{0-\epsilon}^{0+\epsilon} \left(E + \alpha V_o \delta(x) \right) \psi \, dx &= -\frac{2m}{\hbar^2} \left(\int_{0-\epsilon}^{0+\epsilon} E\psi \, dx + \int_{0-\epsilon}^{0+\epsilon} \alpha V_o \delta(x) \psi \, dx \right) \\ &= -\frac{2m}{\hbar^2} \left(0 + \alpha V_o \psi(0) \right) \\ &= -\frac{2m}{\hbar^2} \alpha V_o A \end{aligned}$$

We can now set the two results for Δ equal and simplify:

$$\begin{aligned} -2\kappa A &= -\frac{2m}{\hbar^2} \alpha V_o A \\ -\kappa &= -\frac{m}{\hbar^2} \alpha V_o \\ \kappa^2 &= \frac{m^2 \alpha^2 V_o^2}{\hbar^4} \end{aligned}$$

plugging in κ and solve for the allowed energy values:

$$E = -\frac{m\alpha^2 V_o^2}{2\hbar^2}$$

As all quantities in the expression for E are fixed, the Dirac well of a certain potential evidently only allows for *one* bound state.

6 Finite Square Well

The finite square well potential is given by

$$V(x) = \begin{cases} V_o & |x| \geq a \\ 0 & |x| < a \end{cases}$$

The finite square well bears many similarities to the infinite square well. In particular, we can assume that bound state solutions in the well has the same form as that of the infinite square well, and are alternating between even and odd parities. The major difference is that, now the wave function has two exponential tails extending to infinity on both sides as opposed to simply being 0.

With this knowledge, we can start off by borrowing the result from the infinite well for inside the well. If we label the regions to the left and right of the well by I and III, and inside the well by II, we have:

$$\psi_{II}(x) = A_{II} e^{ikx} + B_{II} e^{-ikx} = C \sin(kx) + D \cos(kx)$$

Then in regions I and III, we have the following equation to solve:

$$\frac{\partial^2}{\partial x^2} \psi(x) = \frac{2m}{\hbar^2} (V_o - E) \psi(x) \equiv \kappa^2 \psi(x)$$

where

$$\kappa \equiv \sqrt{\frac{2m(V_o - E)}{\hbar^2}} \in \mathbb{R}$$

κ is a real number because we assumed that $E < V_o$ (bound state). Solving this equation for regions I and III we obtain:

$$\psi_I(x) = A_I e^{\kappa x} + B_I e^{-\kappa x}$$
$$\psi_{III}(x) = A_{III} e^{\kappa x} + B_{III} e^{-\kappa x}$$

To avoid exponential growth when $x \to \infty$, we set B_I and A_{III} to 0:

$$\psi_I(x) = A_I e^{\kappa x}$$
$$\psi_{III}(x) = B_{III} e^{-\kappa x}$$

We can focus on the even solutions first, so that $C = 0$. The wave function is still required to be continuous at the boundaries, so we have

$$Ae^{-\kappa a} = D\cos(ka) \tag{7}$$
$$Fe^{-\kappa a} = D\cos(ka) \tag{8}$$

We also require the derivatives of the wave function to be continuous at the boundaries:

$$\kappa Ae^{-\kappa a} = kD\sin(ka) \tag{9}$$
$$-\kappa Fe^{-\kappa a} = -kD\sin(ka) \tag{10}$$

Eliminating F with Equations (8) and (10) yields

$$\frac{k}{\kappa} D\sin(ka) = D\cos(ka)$$

rearranging gives a transcendental equation:

$$k\tan(ka) = \kappa$$

If we apply the same logic to the set of odd solutions, we find that

$$k\cot(ka) = -\kappa$$

These transcendental equations have to be solved graphically, and, luckily for us, k and κ obey the following relation:

$$k^2 + \kappa^2 = \frac{2mV_o}{\hbar^2}$$

For graphing convenience, we define $\alpha = ka$ and $\beta = \kappa a$, such that we have these equations to plot:

$$\alpha\tan(\alpha) = \beta$$
$$-\alpha\cot(\alpha) = \beta$$
$$\alpha^2 + \beta^2 = \frac{2mV_o a^2}{\hbar^2} \equiv \gamma^2$$

In words, we are trying to find the intersections of a tangent/cotangent-like graph with a circle of radius γ centered at the origin $(\alpha, \beta) = (0, 0)$. In addition, we are only considering intersections in the first quadrant, since both k and κ are positive values. As the circle gets bigger, more intersections with the tangent/cotangent graphs start to appear — thus more allowed energy eigenstates in the well. This is just as one might expect, since in the infinite well, there is an infinite amount of allowed energy eigenstates. The fact that the even solutions correspond to a graph of tangent also implies that there will **always** be at least one even energy eigenstate no matter how small V_o gets (as long as it is not 0). It is possible for the graph of cotangent, on the other hand, to have no intersection with a circle with center at the origin. In particular, the smallest α-intercept of $-\alpha cot(\alpha)$ in the first quadrant appears at $\alpha = \frac{\pi}{2}$. Therefore, if $\gamma < \frac{\pi}{2}$, then the last odd energy eigenstate will cease to exist. This implies that, in order to have at least one odd energy eigenstate

$$V_o \geq \frac{\pi^2\hbar^2}{8ma^2}$$

has to be true.

7 Harmonic Oscillator

The harmonic oscillator Hamiltonian is given by $H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2$. We then are faced with the following eigenvalue problem:

$$\left(\frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2\right)|E\rangle = E|E\rangle$$

Now, to solve this equation analytically is quite complicated, but thankfully, there is an easier method involving operators due to Dirac.

Let us first define two quantities to make our expressions look nicer:

$$p_o = \sqrt{2\hbar m\omega}$$
$$x_o = \sqrt{\frac{2\hbar}{m\omega}}$$

In terms of these constants, we rewrite H:

$$H = \hbar\omega\left(\frac{P^2}{p_o^2} + \frac{X^2}{x_o^2}\right)$$

The procedure starts with attempting to factor H, as it does have a nice "squared" form:

$$\begin{aligned}
H &\stackrel{?}{=} \hbar\omega\left(\frac{X}{x_o} - i\frac{P}{p_o}\right)\left(\frac{X}{x_o} + i\frac{P}{p_o}\right)\\
H &\stackrel{?}{=} \hbar\omega\left(\frac{X^2}{x_o^2} + i\frac{XP}{x_o p_o} - i\frac{PX}{p_o x_o} + \frac{P^2}{p_o^2}\right)\\
H &\stackrel{?}{=} \hbar\omega\left(\frac{X^2}{x_o^2} + \frac{P^2}{p_o^2} + i\frac{1}{p_o x_o}(XP - PX)\right)\\
H &\stackrel{?}{=} H + i\frac{\hbar\omega}{2\hbar}[X, P]\\
H &\neq H - \frac{1}{2}\hbar\omega
\end{aligned}$$

so we come to the conclusion that H cannot be factored this way, however, this relation is **still** extremely helpful for us. We can rewrite the relation as follows:

$$H = \hbar\omega\left[\left(\frac{X}{x_o} - i\frac{P}{p_o}\right)\left(\frac{X}{x_o} + i\frac{P}{p_o}\right) + \frac{1}{2}\right]$$

We can define the following operators to make this expression look nicer:

$$a = \left(\frac{X}{x_o} + i\frac{P}{p_o}\right) \tag{11}$$

and its adjoint

$$a^\dagger = \left(\frac{X}{x_o} - i\frac{P}{p_o}\right) \tag{12}$$

so that

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) \tag{13}$$

The power of this relation lies in the commutation relations of a, $a^\dagger$, and H. More specifically, as we will see, the commutation relations between $a, a^\dagger$ and H are **self-referential** and will lead to a nice "ladder" structure. The commutation relations are as follows, as one can quickly verify:

$$[a, a^\dagger] = 1, \quad [a^\dagger, a] = -1 \tag{14}$$

and using these one can obtain

$$[a, H] = +\hbar\omega a, \quad [a^\dagger, H] = -\hbar\omega a^\dagger \tag{15}$$

Here is the implication of self-similarity in these commutation relations: **if $|E\rangle$ is an eigenfunction of H, then so is $a|E\rangle$ and $a^\dagger|E\rangle$**. This can be shown as follows:

$$Ha|E\rangle = (aH - \hbar\omega a)|E\rangle$$

where I utilized the commutation relation $[a, H] = +\hbar\omega a$. Then

$$\begin{aligned}(aH - \hbar\omega a)|E\rangle &= (Ea - \hbar\omega a)|E\rangle \\ &= (E - \hbar\omega)a|E\rangle\end{aligned}$$

so we see that $a|E\rangle$ is an eigenfunction of H with eigenvalue $E - \hbar\omega$. Similar logic applies to $a^\dagger$ as well, for which we have:

$$Ha^\dagger|E\rangle = (E + \hbar\omega)|E\rangle$$

This implies the following:

$$\begin{aligned}a|E\rangle &= A|E + \hbar\omega\rangle \\ a^\dagger|E\rangle &= B|E - \hbar\omega\rangle\end{aligned}$$

It is possible to compute A and B for normalized eigenkets. We assume that the eigenkets are normalized to begin with, for which we have:

$$\begin{aligned}\langle aE|aE\rangle &= \langle E|a^\dagger a|E\rangle \\ &= \left\langle E\left|\frac{H}{\hbar\omega} - \frac{1}{2}\right|E\right\rangle \\ &= \left\langle E\left|\frac{E}{\hbar\omega} - \frac{1}{2}\right|E\right\rangle \\ &= \left(\frac{E}{\hbar\omega} - \frac{1}{2}\right)\langle E|E\rangle \\ &= \left(\frac{E}{\hbar\omega} - \frac{1}{2}\right)\end{aligned}$$

but also

$$\langle aE|aE\rangle = A^*A\langle E - \hbar\omega|E - \hbar\omega\rangle = |A|^2$$

so we conclude that, ignoring a phase factor:

$$A = \sqrt{\frac{E}{\hbar\omega} - \frac{1}{2}} \tag{16}$$

it can similarly be shown that

$$B = \sqrt{\frac{E}{\hbar\omega} + \frac{1}{2}} \tag{17}$$

Now we proceed to prove that all energy eigenvalues of the harmonic oscillator H must be non-negative. For an eigenket $|E\rangle$ we have

$$E = \langle E\rangle = \langle E|P^2 + X^2|E\rangle$$

where I have left the constants in H out. Then

$$\begin{aligned}\langle E|P^2 + X^2|E\rangle &= \langle E|P^2|E\rangle + \langle E|X^2|E\rangle \\ &= \langle E|P^\dagger P|E\rangle + \langle E|X^\dagger X|E\rangle \\ &= \langle PE|PE\rangle + \langle XE|XE\rangle \geq 0\end{aligned}$$

where I used the fact that, since X and P are Hermitian. This then must imply that there is a *minimum* rung on this "ladder" of energy eigenvalues. For this minimum eigenket $|E_0\rangle$ we must have that

$$a|E_0\rangle = 0 = A_o|E_0\rangle$$

so $A_o = 0$, using Equation (16) we have that

$$E_0 = \frac{1}{2}\hbar\omega$$

since the $a^\dagger$ operator raises the energy by $\hbar\omega$, we must have a discrete spectrum of energy eigenvalues:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, 3, \ldots \tag{18}$$

We can use this relation to rewrite A and B such that

$$\begin{aligned} a|E\rangle &= \sqrt{n}|E_{n-1}\rangle \\ a^\dagger|E\rangle &= \sqrt{n+1}|E_{n+1}\rangle \end{aligned}$$

notice how $a|E_0\rangle = \sqrt{0}|E_{-1}\rangle = 0$. With this knowledge, we can also express any eigenstate of the harmonic oscillator in terms of the ground state:

$$\begin{aligned} |E_n\rangle &= C_n(a^\dagger)^n|E_0\rangle \\ &= C_n(a^\dagger)^{n-1}\sqrt{1}|E_1\rangle \\ &= C_n(a^\dagger)^{n-2}\sqrt{2}\sqrt{1}|E_2\rangle \\ &= C_n\sqrt{n!}|E_n\rangle \Rightarrow C_n = \frac{1}{\sqrt{n!}} \end{aligned}$$

We can also ignore a factor of $\hbar\omega$ and simply label the energy eigenstates by $|n\rangle$. For previous systems, we were able to directly find energy eigenkets in the X basis. For the harmonic oscillator however, we needed to work around the X basis due to analytic complexity (though possible), so we need to find a way back to the X basis.