II. Applications In One-Dimension

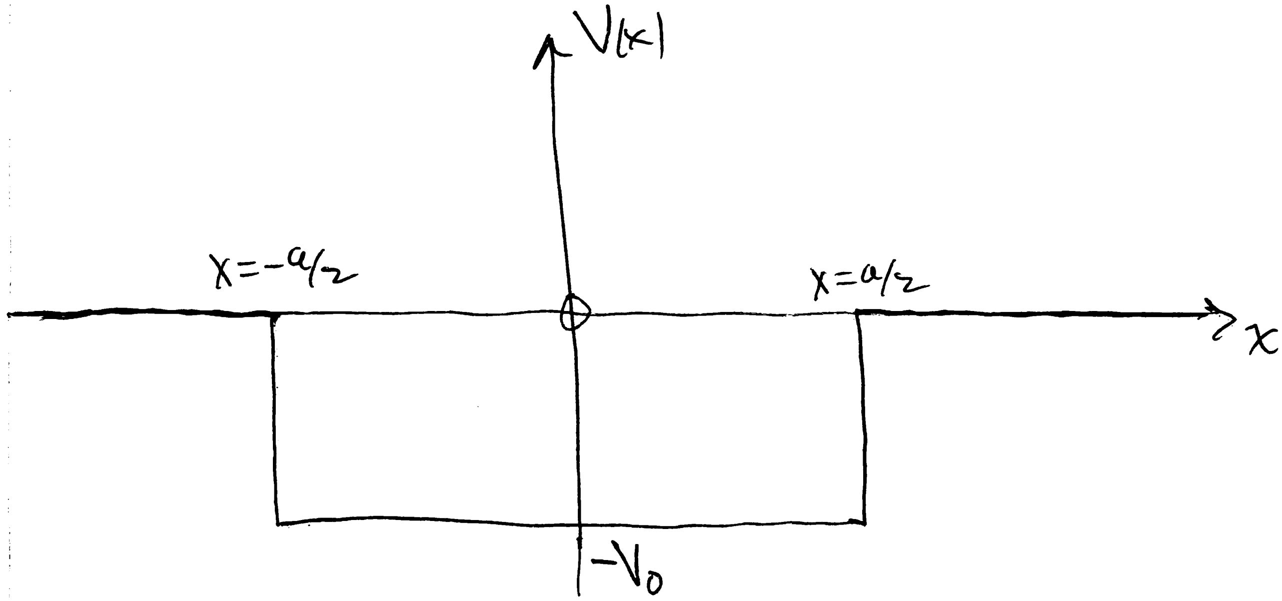
2.2. Bound States

2.2.1. The Square Well

Certain potentials yield solutions to Schrödinger's equation only for certain discrete values of the energy (bound state energies), these are bound states. For example, consider the square well potential in one-dimension given by

$$V(x) = \begin{cases} 0 & , \text{ if } |x| > a/2 \\ -V_0 & , \text{ if } |x| \le a/2 \end{cases}$$

with $V_0 > 0$.



The Schrödinger equation is given by

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\,\psi(x) \qquad , \text{for } |x| > \frac{a}{2}$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) - V_0\psi(x) = E\,\psi(x) \quad , \text{for } |x| \le \frac{a}{2} .$$

We are looking for solutions with negative energy $E<0$ and of course $|E| < V_0$.

Defining

$$\kappa \equiv \sqrt{\frac{2m(-E)}{\hbar^2}} > 0$$

$$q \equiv \sqrt{\frac{2m(E+V_0)}{\hbar^2}} > 0$$

The Schrödinger equation becomes

$$\frac{d^2\psi}{dx^2} - \kappa^2\psi = 0 \qquad , \text{for } |x| > \frac{a}{2}$$

$$\frac{d^2\psi}{dx^2} + q^2\psi = 0 \qquad , \text{for } |x| \le a/2 .$$

As usual the general solution to this differential equation is

$$\psi(x)=\begin{cases} A_< e^{\kappa x} + B_< e^{-\kappa x}, & \text{for } x<-\frac{a}{2} \\ A e^{iqx} + B e^{-iqx}, & \text{for } -\frac{a}{2}\le x\le\frac{a}{2} \\ A_> e^{\kappa x} + B_> e^{-\kappa x}, & \text{for } x>\frac{a}{2}. \end{cases}$$

The boundary conditions on ψ & ψ' will further determine the solution we desire

1) ψ is finite everywhere

For $x\to-\infty \Rightarrow B_< = 0$

For $x\to+\infty \Rightarrow A_> = 0$

2) Continuity of ψ and $\frac{d\psi}{dx}$ at $x=-\frac{a}{2}$

$\psi(-\frac{1}{2}a^-)=\psi(-\frac{1}{2}a^+)\Rightarrow$

$$A_< e^{-\kappa\frac{a}{2}} = A e^{-iq\frac{a}{2}} + B e^{iq\frac{a}{2}}$$

$\psi'(-\tfrac{1}{2}a^-) = \psi'(-\tfrac{1}{2}a^+) \Rightarrow$

$$\kappa A_< e^{-\kappa\frac{a}{2}} = iq\left(A e^{-iq\frac{a}{2}} - B e^{+iq\frac{a}{2}}\right)$$

Combining these we have

$$\boxed{\begin{aligned} A &= \tfrac{1}{2}\left(1+\frac{\kappa}{iq}\right)e^{(iq-\kappa)\frac{a}{2}}A_< \\ B &= \tfrac{1}{2}\left(1-\frac{\kappa}{iq}\right)e^{(-iq-\kappa)\frac{a}{2}}A_< . \end{aligned}}$$

3) Continuity of ψ and $\frac{d\psi}{dx}$ at $x=+\frac{a}{2}$

$\psi(\tfrac{1}{2}a^-) = \psi(\tfrac{1}{2}a^+) \Rightarrow$

$$B_> e^{-\kappa\frac{a}{2}} = A e^{iq\frac{a}{2}} + B e^{-iq\frac{a}{2}}$$

$\psi'(\tfrac{1}{2}a^-) = \psi'(\tfrac{1}{2}a^+) \Rightarrow$

$$-\kappa B_> e^{-\kappa\frac{a}{2}} = iq\left(A e^{iq\frac{a}{2}} - B e^{-iq\frac{a}{2}}\right)$$

Substituting for A and B from case 2 we find 2 expressions for the same $B_>$

$$\boxed{\begin{aligned} B_> &= \left[\tfrac{1}{2} e^{iqa}\left(1+\frac{\kappa}{iq}\right) + \tfrac{1}{2} e^{-iqa}\left(1-\frac{\kappa}{iq}\right)\right] A_< \\ B_> &= \frac{-iq}{2\kappa}\left[\tfrac{1}{2} e^{iqa}\left(1+\frac{\kappa}{iq}\right) - \tfrac{1}{2} e^{-iqa}\left(1-\frac{\kappa}{iq}\right)\right] A_< . \end{aligned}}$$

Thus for a non-trivial ψ to exist, we must have both expressions for $B_>$ to be equal

$$\frac{1}{2}\left[e^{iqa}\left(1+\frac{\kappa}{iq}\right) + e^{-iqa}\left(1-\frac{\kappa}{iq}\right)\right]$$

$$= \frac{-iq}{2\kappa}\left[e^{iqa}\left(1+\frac{\kappa}{iq}\right) - e^{-iqa}\left(1-\frac{\kappa}{iq}\right)\right]$$

$$\Rightarrow \quad \boxed{e^{2iqa} = \left(\frac{\kappa - iq}{\kappa + iq}\right)^2}$$

Since κ and q depend on E, this equation will lead to discrete allowed values for the bound state energies E. Since the right hand side is a square, there are 2 cases

Case 1)

$$-e^{iqa} = \frac{\kappa - iq}{\kappa + iq}$$

Case 2)

$$+e^{iqa} = \frac{\kappa - iq}{\kappa + iq}.$$

Case 1)

$$-e^{+iqa} = \frac{\kappa - iq}{\kappa + iq} \Rightarrow \boxed{\frac{\kappa}{q} = \tan\frac{qa}{2}}$$

Since $\kappa > 0$, $q > 0$ this also implies $\boxed{\tan\frac{qa}{2} > 0.}$

Defining

$$q_0 \equiv \sqrt{q^2 + \kappa^2} = \sqrt{\frac{2mV_0}{\hbar^2}}$$

we see that the above is simply

$$\tan^2\frac{qa}{2} = \sec^2\frac{qa}{2} - 1 = \frac{\kappa^2}{q^2}$$

or

$$\kappa^2 + q^2 = q^2\frac{1}{\cos^2\frac{qa}{2}}$$

$$\Rightarrow \quad \cos^2\frac{qa}{2} = \frac{q^2}{q_0^2} \qquad \text{since } q > 0$$

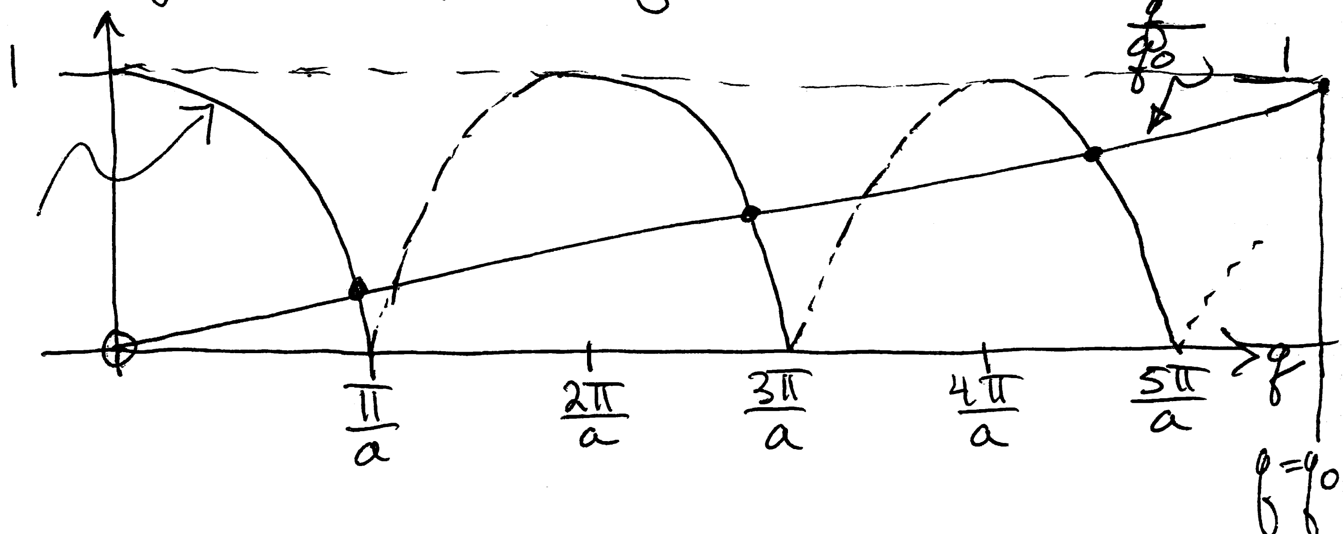
we find $\boxed{\left|\cos\frac{qa}{2}\right| = \frac{q}{q_0}}$

In order to solve the transcendental equations

$$\left|\cos\frac{qa}{2}\right| = \frac{q}{q_0} \quad ; \quad \tan\frac{qa}{2} > 0 \,,$$

we graph the functions $\frac{q}{q_0}$ and $\left|\cos\frac{qa}{2}\right|$ and find the points of intersection

$\left|\cos\frac{qa}{2}\right|$



The solid $\left|\cos\frac{qa}{2}\right|$ curve lines also have $\tan\frac{qa}{2} > 0$. The dashed lines correspond to $\tan\frac{qa}{2} < 0$, and are excluded in case 1 solutions. The intersection of $\frac{q}{q_0}$ with $\left|\cos\frac{qa}{2}\right|$ indicated by the dots, are the allowed solutions q to the transcendental equation. In the case drawn here we have for the q_0 indicated 3 allowed bound states in case 1.

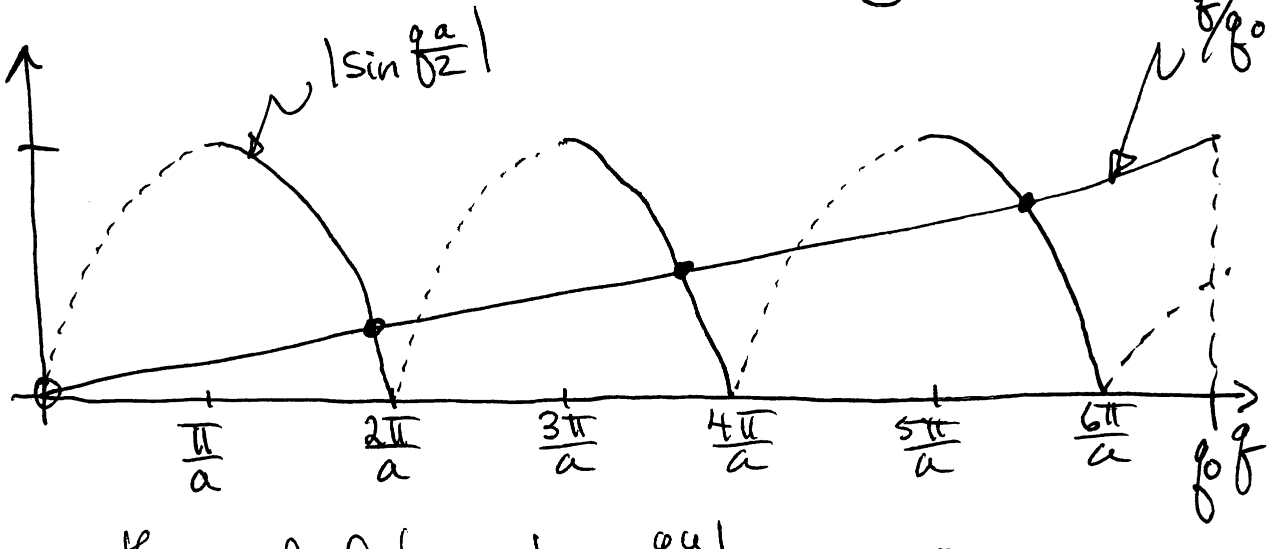
Case 2) $+e^{iqa} = \frac{\kappa - iq}{\kappa + iq} \Rightarrow \boxed{-\frac{q}{\kappa} = \tan\frac{qa}{2}}$

Since $q > 0, \kappa > 0 \Rightarrow \boxed{\tan\frac{qa}{2} < 0}$.

Using $q_0 = \sqrt{q^2+\kappa^2} = \sqrt{\frac{2mV_0}{\hbar^2}}$ again, this becomes

$$\boxed{\left|\sin\frac{qa}{2}\right| = \frac{q}{q_0} \text{ and } \tan\frac{qa}{2} < 0}$$

The graphical solution is given by



Again, the solid line $|\sin\frac{qa}{2}|$ curve is that part for which $\tan qa/2 < 0$ also. The intersection of this curve with q/q_0 are the allowed values of q and hence E, the bound state energies. The

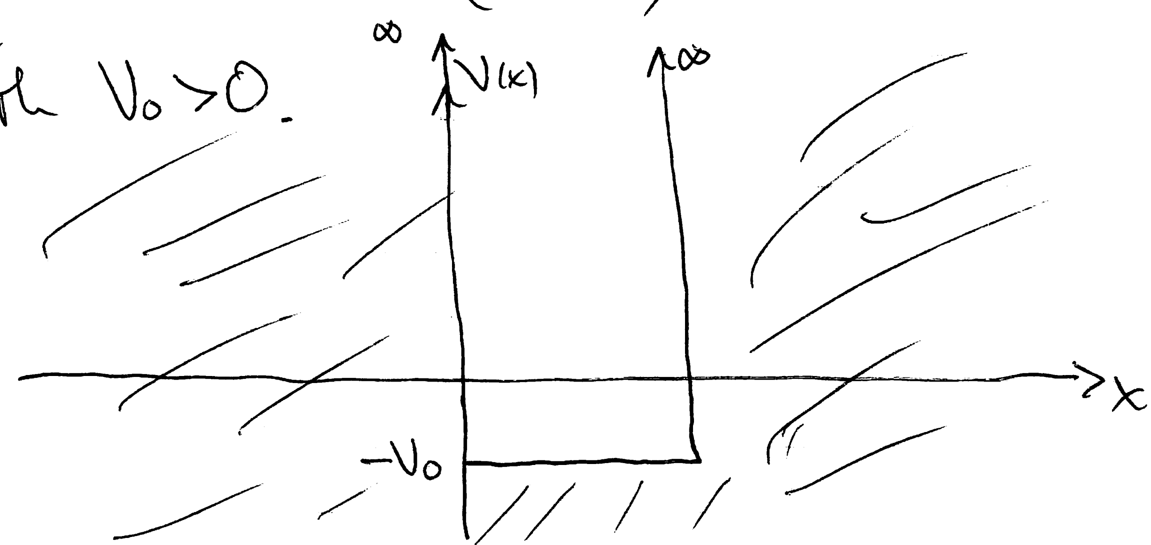
Solution to the bound state problem of our square well consists of both sets of these intersection points. Only discrete (quantized) values of the energy E lead to allowed solutions.

We can also consider the case where the potential well is infinitely deep. Can see that as $V_0 \to \infty$ $q/q_0 \to 0$ thus the allowed solutions will have $|\sin\frac{qa}{2}| = 0 = |\cos\frac{qa}{2}|$ that is $\frac{qa}{2} = \frac{n\pi}{2}$, $n = 1, 2, 3, \ldots$ that is the allowed values of q are $q_n = \frac{n\pi}{a}$, $n = 1, 2, \ldots$
Rather than take the $V_0 \to \infty$ limit above we can solve this infinite square well problem directly.

Consider the one-dimensional potential

$$V(x) = \begin{cases} \infty , & x < 0 \\ -V_0 , & 0 \le x \le a \\ \infty , & x > a \end{cases}$$

with $V_0 > 0$.



As we discussed in section 1.3.8, for infinitely high potential walls the wave function is zero inside the walls, physically it is clear that the infinite potential wall prevents any probability of finding the particle in that region. Thus

$$\psi(x) = 0 \quad \text{for } x \leq 0 \text{ and } x \geq a .$$

Inside the well the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi \quad , \text{for } 0<x<a,$$

with the boundary conditions

$$\psi(0) = 0 = \psi(a) .$$

Letting $q \equiv \sqrt{\frac{2m(E+V_0)}{\hbar^2}} > 0$, the Schrödinger equation becomes

$$\frac{d^2}{dx^2}\psi + q^2\psi = 0 \quad , \quad 0 \leq x \leq a .$$

In general

$$\psi(x) = A\cos qx + B\sin qx \quad , \quad 0 \leq x \leq a .$$

Applying the BC implies

1) $\psi(0)=0 \Rightarrow A=0$

2) $\psi(a)=0 \Rightarrow B\sin qa=0$.

Since $B=0$ is just the trivial solution which is unphysical, it follows that q can only take on discrete allowed values of

$$q_n=\frac{n\pi}{a}\,,\quad n=1,2,3,\ldots\,.$$

Hence

$$\psi_n(x)=B_n\sin q_n x=B_n\sin\frac{n\pi x}{a}$$

with $n=1,2,3,\ldots$ for $0\le x\le a$.

Note, $n=0$ implies $\psi=0$, which we have excluded on physical grounds — the particle must be somewhere. Finally we can choose to normalize the wavefunction to 1

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

$$=|B_n|^2\int_0^a dx\,\sin^2\frac{n\pi x}{a}$$

for $\theta=\frac{n\pi x}{a}$ we find

$$1 = |B_n|^2 \frac{a}{n\pi} \int_0^{n\pi} d\theta \sin^2\theta$$

$$= |B_n|^2 \frac{a}{n\pi} \; n \underbrace{\int_0^{\pi} d\theta \sin^2\theta}_{=\pi/2}$$

$$\Rightarrow \quad 1 = |B_n|^2 \frac{a}{2} \quad \text{or} \quad |B_n|^2 = \frac{2}{a} .$$

Choosing B_n to be real and positive we have

$$B_n = \sqrt{\frac{2}{a}} .$$

Thus

$$\psi_n(x) = \begin{cases} 0 & , \text{ for } x < 0 \\ \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} & , \text{ for } 0 \leq x \leq a \\ 0 & , \text{ for } x > a . \end{cases}$$

These are the energy eigenfunctions for the infinite square well potential with bound state energies

$$E_n = \frac{\hbar^2}{2m} q_n^2 - V_0$$

i.e. $q^2 = \frac{2m(E+V_0)}{\hbar^2}$

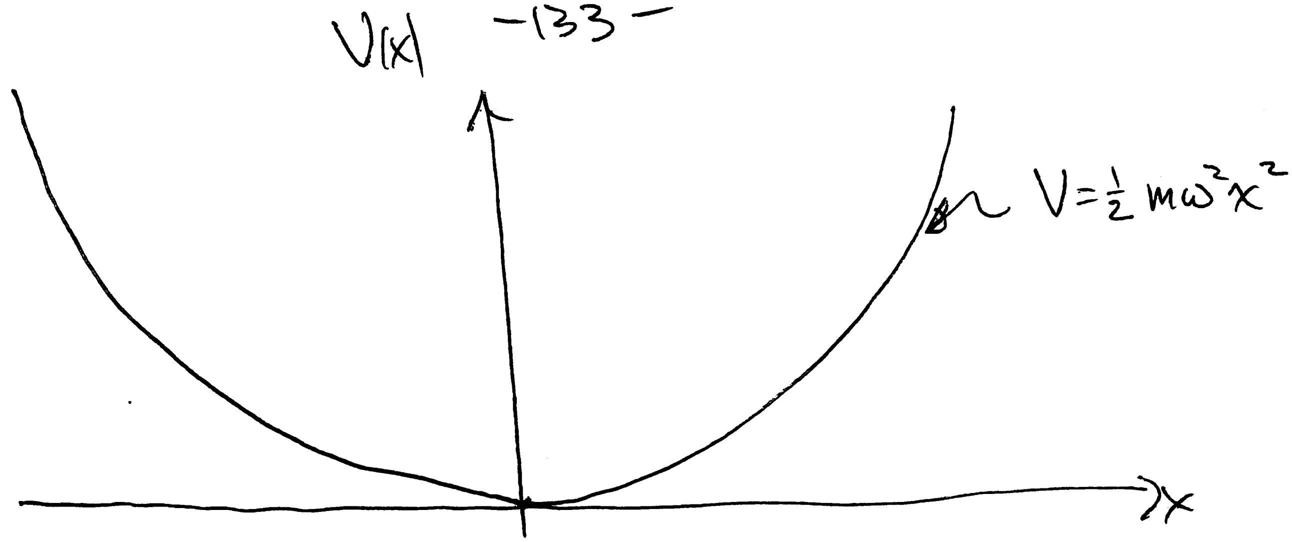
$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2 - V_0$$
$$= \frac{\hbar^2\pi^2}{2ma^2}\, n^2 - V_0 \qquad , \; n = 1, 2, 3, \ldots$$

2.2.2. The Simple Harmonic Oscillator

As in classical mechanics, the quantum mechanical simple harmonic oscillator (SHO) is an extremely important example since it can be used to describe the behavior of systems undergoing small oscillations. In addition such a framework appears in quantum field theory where the oscillations correspond to the creation and annihilation of free particles.
The SHO is defined in 1-dimension to have the potential

$$V(x) = \tfrac{1}{2} m\omega^2 x^2$$

with m the mass of the particle and ω a constant here.



The Schrödinger equation for a particle moving in this potential is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + \frac{1}{2}m\omega^2 x^2 \psi = E\psi .$$

It is convenient to introduce dimensionless variables in order to solve the differential equation

$$\epsilon \equiv \frac{E}{\hbar\omega} \quad \text{and} \quad \xi \equiv \sqrt{\frac{m\omega}{\hbar}}\, x .$$

The Schrödinger equation becomes

$$\frac{d^2}{d\xi^2}\varphi(\xi) + (2\epsilon - \xi^2)\varphi(\xi) = 0$$

where $\qquad \varphi(\xi) = \psi(x).$

This equation can be solved by familiar power series methods. Rather than proceed this way we notice that

$$\left(\frac{\partial}{\partial\xi}+\xi\right)\left(\frac{\partial}{\partial\xi}-\xi\right)\varphi(\xi)=\left(\frac{\partial^2}{\partial\xi^2}-\xi^2-1\right)\varphi(\xi).$$

Hence the Schrödinger equation can be written

$$\left(\frac{\partial}{\partial\xi}+\xi\right)\left(\frac{\partial}{\partial\xi}-\xi\right)\varphi(\xi)=\left[-2\epsilon-1\right]\varphi(\xi).$$

Alternatively, we can write the equation as

$$\left(\frac{\partial}{\partial\xi}-\xi\right)\left(\frac{\partial}{\partial\xi}+\xi\right)\varphi(\xi)=\left[-2\epsilon+1\right]\varphi(\xi)$$

Multiplying the first expression by $\left(\frac{\partial}{\partial\xi}-\xi\right)$ yields

$$\left(\frac{\partial}{\partial\xi}-\xi\right)\left(\frac{\partial}{\partial\xi}+\xi\right)\left[\left(\frac{\partial}{\partial\xi}-\xi\right)\varphi(\xi)\right]$$
$$=\left[-2\epsilon-1\right]\left[\left(\frac{\partial}{\partial\xi}-\xi\right)\varphi(\xi)\right]$$

This can be true if either

$$\left(\frac{\partial}{\partial\xi}-\xi\right)\varphi(\xi)=0$$

or

$$\left(\frac{\partial}{\partial\xi}-\xi\right)\varphi(\xi) \equiv \varphi'(\xi) \quad \text{such that}$$

$$\left(\frac{\partial}{\partial\xi}-\xi\right)\left(\frac{\partial}{\partial\xi}+\xi\right)\varphi'(\xi) = [-2\epsilon-1]\varphi'(\xi).$$

But this equation is nothing but the other form of writing the Schrödinger equation

$$\left(\frac{\partial}{\partial\xi}-\xi\right)\left(\frac{\partial}{\partial\xi}+\xi\right)\varphi'(\xi) = [-2\epsilon'+1]\varphi'(\xi)$$

with $\epsilon' = \epsilon+1$, so given eigenfunction $\varphi(\xi)$ we find eigenfunction φ' with eigenvalue $\epsilon'=\epsilon+1$.

Now if its the first case, $\left(\frac{\partial}{\partial\xi}-\xi\right)\varphi(\xi)=0$, we have that $\varphi(\xi)=Ne^{+\frac{1}{2}\xi^2}$. But $\psi(x)$ must be finite and normalizable, as $\xi\to\infty$ $\varphi(\xi)\to\infty$ thus, this solution is ruled out by the boundary conditions on $\psi(x)$. Hence we have the second case; given any solution $\varphi(\xi)$ with eigenvalue ϵ we can generate a new eigenfunction $\varphi'(\xi)$ by

$$\varphi'(\xi) = \left(\frac{\partial}{\partial\xi}-\xi\right)\varphi(\xi),$$

with eigenvalue $\epsilon'=\epsilon+1$.

Analogously we multiply the second form of Schrödinger's equation by $\left(\frac{\partial}{\partial\xi}+\xi\right)$

$$\left(\frac{\partial}{\partial\xi}+\xi\right)\left(\frac{\partial}{\partial\xi}-\xi\right)\left(\frac{\partial}{\partial\xi}+\xi\right)\varphi(\xi)$$

$$=\left[-2\epsilon+1\right]\left(\frac{\partial}{\partial\xi}+\xi\right)\varphi(\xi).$$

This is true if either

$$\left(\frac{\partial}{\partial\xi}+\xi\right)\varphi(\xi)=0$$

or

$$\varphi''(\xi)\equiv\left(\frac{\partial}{\partial\xi}+\xi\right)\varphi(\xi)$$

with

$$\left(\frac{\partial}{\partial\xi}+\xi\right)\left(\frac{\partial}{\partial\xi}-\xi\right)\varphi''(\xi)=\left[-2\epsilon''+1\right]\varphi''(\xi)$$

where $\epsilon''=\epsilon-1$. So we see that given any eigenfunction $\varphi(\xi)$ with eigenvalue ϵ, we can always generate a new eigenfunction $\varphi''(\xi)$ by

$$\varphi''(\xi)=\left(\frac{\partial}{\partial\xi}+\xi\right)\varphi(\xi)\quad\text{with}$$

a lower energy eigenvalue $\epsilon''=\epsilon-1$.

However the Hamiltonian is a non-negative operator $H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 x^2$. That is given any wavefunction $\psi(x,t)$ we have

$$\int_{-\infty}^{+\infty} d\xi \; \varphi^*(\xi,t)\left(-\frac{\partial}{\partial\xi}+\xi\right)\left(\frac{\partial}{\partial\xi}+\xi\right)\varphi(\xi,t)$$

$$= \int_{-\infty}^{+\infty} d\xi \left[\left(\frac{\partial}{\partial\xi}+\xi\right)\varphi\right]^* \left(\frac{\partial}{\partial\xi}+\xi\right)\varphi$$

$$= \int_{-\infty}^{+\infty} d\xi \left|\left(\frac{\partial}{\partial\xi}+\xi\right)\varphi\right|^2 \geq 0 .$$

This implies that the eigenvalues of

$\left(-\frac{\partial}{\partial\xi}+\xi\right)\left(\frac{\partial}{\partial\xi}+\xi\right)$ must be non-negative

But $\left(-\frac{\partial}{\partial\xi}+\xi\right)\left(\frac{\partial}{\partial\xi}+\xi\right)\varphi(\xi) = [2\epsilon-1]\varphi(\xi)$

hence for all eigenfunctions $\varphi(\xi)$ the eigenvalue

$$2\epsilon - 1 \geq 0, \text{ that is}$$

$$\boxed{\epsilon \geq \frac{1}{2}} .$$

So if we continue to let $\left(\frac{\partial}{\partial\xi}+\xi\right)$ act on $\varphi(\xi)$ we will lower the eigenvalue ϵ by 1 each time

φ has eigenvalue ϵ

$\varphi^{(1)} = \left(\frac{\partial}{\partial \xi} + \xi\right) \varphi(\xi)$ has eigenvalue $\epsilon - 1$

$\varphi^{(2)} = \left(\frac{\partial}{\partial \xi} + \xi\right)^2 \varphi(\xi)$ has eigenvalue $\epsilon - 2$

$\vdots$

$\varphi^{(n)} = \left(\frac{\partial}{\partial \xi} + \xi\right)^n \varphi(\xi)$ has eigenvalue $\epsilon - n$,

eventually n will be large enough so that

$(2\epsilon - 1) - n < 0$. But this is forbidden since H is non-negative. Thus there exists some power of n such that one more application of $\left(\frac{\partial}{\partial \xi} + \xi\right)$ causes the function to vanish; that is there exists an n

$$\varphi_0(\xi) \equiv \left(\frac{\partial}{\partial \xi} + \xi\right)^n \varphi(\xi)$$

so that

$$\left(\frac{\partial}{\partial \xi} + \xi\right) \varphi_0(\xi) = 0 .$$

This is nothing but the other choice in this case. So we see that we can always generate a lower energy eigenfunction by action of $\left(\frac{\partial}{\partial \xi} + \xi\right)$ on $\varphi(\xi)$ unless $\varphi(\xi)$ is the ground state $\varphi_0(\xi)$.

In that case

$$\left(\frac{\partial}{\partial\xi}+\xi\right)\varphi_0(\xi)=0 \quad . \text{ Since}$$

this is a 1st order differential equation
the solution is
unique $\boxed{\varphi_0(\xi) = N_0 e^{-\frac{1}{2}\xi^2}}$ with

N_0 a normalization constant. Further
Since $\left(\frac{\partial}{\partial\xi}+\xi\right)\varphi_0(\xi)=0$ we have

$$0=\left(\frac{\partial}{\partial\xi}-\xi\right)\left(\frac{\partial}{\partial\xi}+\xi\right)\varphi_0(\xi)=\left[-2\epsilon_0+1\right]\varphi_0(\xi)$$

$\Rightarrow$

$\epsilon_0 = \frac{1}{2}$, the ground state,

the state with lowest energy eigenvalue,
has energy $\boxed{\epsilon_0 = \frac{1}{2} \text{ or } E_0 = \frac{1}{2}\hbar\omega}$.

Starting from the ground state, all
other eigenfunctions and eigenvalues
can be reached by action of $\left(\frac{\partial}{\partial\xi}-\xi\right)$
on the $\varphi_0(\xi)$. Since each state will
correspond to raising the energy by 1
we have that the spectrum of energies

For the SHO is labelled by an integer

$$\epsilon_n = n + \tfrac{1}{2} \quad ; \quad n = 0, 1, 2, 3, \ldots$$

Thus the energy eigenvalues are

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

The n^{th} excited state eigenfunction φ_n is simply

$$\varphi_n(\xi) = \frac{N_n}{N_0}\left(\frac{\partial}{\partial \xi} - \xi\right)^n \varphi_0(\xi) \quad .$$

Hence

$$\varphi_0 = N_0 \, e^{-\frac{1}{2}\xi^2}$$

$$\varphi_1 = N_1(-2\xi)e^{-\frac{1}{2}\xi^2}$$

$$\varphi_2 = N_2 \, 2(2\xi^2 - 1)e^{-\frac{1}{2}\xi^2}$$

$$\varphi_3 = N_3(-4)(2\xi^3 - 3\xi)e^{-\frac{1}{2}\xi^2}$$

$$\vdots$$

Note: $\varphi_0 = \left(\frac{\partial}{\partial\xi}+\xi\right)^n \varphi$ thus we have

$$\left(\frac{\partial}{\partial\xi}+\xi\right)\left(\frac{\partial}{\partial\xi}-\xi\right)\varphi_0 = [-2\epsilon + 2n \ominus 1]\varphi_0$$

but $\left[\left(\frac{\partial}{\partial\xi}+\xi\right), \left(\frac{\partial}{\partial\xi}-\xi\right)\right] = -2$

$$\Rightarrow \quad [-2\epsilon + 2n \cancel{+3} + 1]\varphi_0 = 0$$

$$\Rightarrow \quad \epsilon = n + \frac{\cancel{3}}{2}\ \frac{1}{2}$$ since $n = 0, 1, 2, \dots$

we see that the totality of eigenvalues is given by $\epsilon_n = n + \frac{1}{2}$, $n = 0, 1, 2, \dots$, that is odd half-integers.

Now we recognize the eigenfunctions as just the Hermite polynomials times $e^{-\frac{1}{2}\xi^2}$.

$$\boxed{H_n(\xi) \equiv (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2}}$$

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

Notice that

$$\frac{d^n}{d\xi^n} e^{-\xi^2} = \frac{d^n}{d\xi^n} e^{-\frac{1}{2}\xi^2} e^{-\frac{1}{2}\xi^2}$$

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

Continuing,

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

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

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

Recall
$$\varphi_n(\xi) = \frac{N_n}{N_0} \left(\frac{d}{d\xi} - \xi\right)^n \varphi_0(\xi)$$

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

$$\boxed{\varphi_n(\xi) = N_n (-1)^n H_n(\xi) e^{-\frac{1}{2}\xi^2}}$$

Recalling that $\xi = \sqrt{\frac{m\omega}{\hbar}}\, x$ and $\psi(x) = \varphi(\xi)$ we have the energy eigenfunctions

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

with corresponding eigenvalues $E_n = (n + \frac{1}{2})\hbar\omega$ for $n = 0, 1, 2, \ldots$.

Let's Review some of the properties of the Hermite Polynomials $H_n(\xi)$:

1) $H_n(-\xi) = (-1)^n H_n(\xi)$; $H_n(\xi)$ is an even (odd) function of ξ for n even (odd).

2) $H_n(\xi)$ obey the differential equation

$$\left[\frac{d^2}{d\xi^2} - 2\xi\frac{d}{d\xi} + 2n\right] H_n(\xi) = 0$$

3) $H_n(\xi)$ can be obtained from the generating function $Z(s)$ by differentiation

$$Z(s) \equiv \sum_{n=0}^{\infty} \frac{s^n}{n!} H_n(\xi)$$

$$= e^{-s^2+2s\xi}$$

Thus $$H_n(\xi) = \frac{\partial^n}{\partial s^n} Z(s) \Big|_{s=0} .$$

4) Recursion Relations

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

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

these follow most easily from $Z(s)$ ex.

$$\frac{\partial Z}{\partial \xi} = \sum_{n=0}^{\infty} \frac{s^n}{n!} \frac{d H_n(\xi)}{d\xi}$$

$$= 2s\, Z(s)$$

$$= 2 \sum_{m=0}^{\infty} \frac{s^{m+1}}{m!} H_m(\xi) \quad \text{let } n = m+1$$

$$= 2 \sum_{n=1}^{\infty} \frac{s^n\, n}{(n-1)!\, n} H_{n-1}(\xi)$$

$$= \sum_{n=1}^{\infty} \frac{s^n}{n!} 2n H_{n-1}(\xi)$$

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

5) $H_n^*(\xi) = H_n(\xi)$; $H_n(\xi)$ are real.

6) Low order Hermite Polynomials

$H_0 = 1$ $\qquad$ $H_n(\xi)$ is a n^{th} order polynomial in ξ

$H_1 = 2\xi$

$H_2 = 4\xi^2 - 2$

$H_3 = 8\xi^3 - 12\xi$

$\vdots$

7) The Hermite Polynomials are orthogonal wrt $e^{-\xi^2}$

$$\boxed{\int_{-\infty}^{+\infty} d\xi\, e^{-\xi^2} H_m(\xi) H_n(\xi) = \delta_{mn} 2^n n! \sqrt{\pi}}$$

Proof: consider $m \geq n$

$$\int_{-\infty}^{+\infty} d\xi\, e^{-\xi^2} H_m(\xi) H_n(\xi)$$

$$= \int_{-\infty}^{+\infty} d\xi\, \cancel{e^{-\xi^2}} (-1)^{m+n} \left[\cancel{e^{\xi^2}} \frac{d^m}{d\xi^m} e^{-\xi^2}\right]\left[e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2}\right]$$

$$= (-1)^{m+n} \int_{-\infty}^{+\infty} d\xi \left(\frac{d^m}{d\xi^m} e^{-\xi^2}\right)\left(e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2}\right)$$

Now integrate the first term by parts m-times throwing away the "surface" terms since $\xi^l e^{-\xi^2} \to 0$ as $\xi \to \pm\infty$

$$= (-1)^{2m+n} \int_{-\infty}^{+\infty} d\xi\, e^{-\xi^2} \frac{d^m}{d\xi^m} \underbrace{\left(e^{+\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2}\right)}_{\substack{n^{th}\text{ degree polynomial} \\ h_n \xi^n + h_{n-1} \xi^{n-1} + \cdots + h_0}}$$

but $m \geq n$ thus the $m^{\underline{th}}$ derivative vanishes unless $m=n$, then only the $\underline{h_n m!}$ term survives. From

$$Z(s) = e^{-s^2+2s\xi} \quad \text{and} \quad H_n(\xi) = \frac{\partial^n}{\partial s^n} Z(s)\Big|_{s=0}$$

we see that the $h_n \xi^n$ term comes from the $n^{\underline{th}}$ s-derivative on $e^{2s\xi}$ thus $h_n = (-2)^n$, i.e. $H_n(\xi) = (2)^n \xi^n + O(\xi^{n-2})$

So
$$\int_{-\infty}^{+\infty} d\xi\, e^{-\xi^2} H_m(\xi) H_n(\xi)$$
$$= \delta_{mn} (-1)^n \int_{-\infty}^{+\infty} d\xi\, e^{-\xi^2} (-2)^n n!$$

but
$$\int_{-\infty}^{+\infty} d\xi\, e^{-\xi^2} = \sqrt{\pi}$$

Thus we obtain the desired result

$$\int_{-\infty}^{+\infty} d\xi\, e^{-\xi^2} H_m(\xi) H_n(\xi) = \delta_{mn} 2^n n! \sqrt{\pi}$$

From this property we can determine the normalization of the energy eigenfunctions

$$\int_{-\infty}^{+\infty} dx\, \psi_m^*(x)\, \psi_n(x)$$

$$= N_m^* N_n (-1)^{m+n} \int_{-\infty}^{+\infty} dx\, H_m(\xi) e^{-\frac{1}{2}\xi^2} H_n(\xi)\, e^{-\frac{1}{2}\xi^2}$$

recalling $\xi = \sqrt{\frac{m\omega}{\hbar}}\, x$

$$= N_m^* N_n (-1)^{m+n} \sqrt{\frac{\hbar}{m\omega}} \int_{-\infty}^{+\infty} d\xi\, e^{-\xi^2} H_m(\xi) H_n(\xi)$$

$$= \delta_{mn} |N_n|^2\, 2^n\, n! \left(\frac{\hbar\pi}{m\omega}\right)^{1/2}$$

Thus we can make the wavefunctions orthonormal by choosing

$$N_n = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} \left(\frac{1}{2^n n!}\right)^{1/2} e^{in\pi}$$

where $e^{in\pi} = (-1)^n$, the phase of N_n, is chosen to eliminate the $(-1)^n$ factor in $\psi_n(x)$ by convention.

To Summarize: The orthonormal energy eigenfunctions ψ_n, with eigenvalues E_n, for the SHO in one-dimension

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega^2x^2\right]\psi_n(x)=E_n\psi_n(x)$$

are given by

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

with H_n the n^{th} order Hermite polynomial and

$$E_n=(n+\tfrac{1}{2})\hbar\omega \qquad \text{for } n=0,1,2,\ldots$$

Note: the ground state, $n=0$, has energy $E_0=\frac{1}{2}\hbar\omega$, the zero-point energy of the SHO. Also the wavefunctions form a complete set of states

$$\sum_{n=0}^{\infty}\psi_n^*(y)\psi_n(x)=\delta(x-y),$$

and are orthonormal

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

Having solved the eigenvalue equation for the 1-dimensional SHO, it is straightforward to solve the p-dimensional isotropic SHO
same ω for each $x_i \Leftrightarrow$ isotropic

$$\underbrace{\left[-\frac{\hbar^2}{2m}\sum_{i=1}^{p}\frac{d^2}{dx_i^2}+\frac{1}{2}m\omega^2 x_i^2\right]}_{\equiv H}\psi_{n_1\cdots n_p}(x_1,\dots,x_p) = E_n\psi_{n_1\cdots n_p}(x_1,\dots,x_p)$$

where
$$H=\sum_{i=1}^{p} H_i$$
and the H_i are just the 1-dimensional SHO's for the x_i - coordinate

$$H_i = -\frac{\hbar^2}{2m}\frac{d^2}{dx_i^2}+\frac{1}{2}m\omega^2 x_i^2 .$$

Hence the solution $\psi_{n_1\cdots n_p}$ is just the product of 1dimensional SHO wavefunctions (separation of variables since $H=\sum_i H_i$ and $[H_i,H_j]=0$)

$$\psi_{n_1\cdots n_p}(x_1,\dots,x_p) = \psi_{n_1}(x_1)\cdots\psi_{n_p}(x_p)$$

where
$$H_i\psi_{n_i}(x_i) = E_{n_i}\psi_{n_i}(x_i) .$$

Thus
$$H\psi_{n_1\cdots n_p} = (E_{n_1}+\cdots+E_{n_p})\psi_{n_1\cdots n_p}$$
$$\equiv E_n\psi_{n_1\cdots n_p}$$

The p-dimensional energy eigenvalues are

$$E_n = (n_1 + \cdots + n_p + \tfrac{p}{2})\hbar\omega = (n + \tfrac{p}{2})\hbar\omega$$

where $n = n_1 + \cdots + n_p$.

The complete set of eigenfunctions $\psi_{n_1 \cdots n_p}$ are labelled by p-integers $n_1, \ldots, n_p$ each of which range from 0 to ∞. The energy eigenvalues on the other hand depend only on the sum of these integers $n = n_1 + n_2 + \cdots + n_p$. For a given $n \geq 0$ there exists

$$C^{n}_{n+p-1} = \frac{(n+p-1)!}{n!\,(p-1)!} \quad \text{distinct}$$

values for $(n_1, n_2, \ldots, n_p)$ such that their sum is n. (This is just the number of ways for $(n_1, \ldots, n_p)$ to add up to n; it is equal to the number of different ways of putting n-identical objects into p-boxes i.e. putting n-balls into p boxes

$$= \frac{(n+p-1)!}{n!\,(p-1)!}$$

Hence E_n is C^{n}_{n+p-1}-fold degenerate.

For example consider $p=3$; the 3-dimensional isotropic SHO $H = H_x + H_y + H_z$,

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + \frac{1}{2}m\omega^2(x^2+y^2+z^2)$$

$$\psi_{n_x n_y n_z}(\vec{r}) = \psi_{n_x}(x)\psi_{n_y}(y)\psi_{n_z}(z) \quad \text{and}$$

$$\begin{aligned}
H\psi_{n_x n_y n_z} &= (H_x + H_y + H_z)\psi_{n_x}(x)\psi_{n_y}(y)\psi_{n_z}(z) \\
&= [H_x\psi_{n_x}(x)]\psi_{n_y}(y)\psi_{n_z}(z) \\
&\quad + \psi_{n_x}(x)[H_y\psi_{n_y}(y)]\psi_{n_z}(z) \\
&\quad + \psi_{n_x}(x)\psi_{n_y}(y)[H_z\psi_{n_z}(z)] \\
&= (E_{n_x} + E_{n_y} + E_{n_z})\psi_{n_x}(x)\psi_{n_y}(y)\psi_{n_z}(z) \\
&= (n_x + n_y + n_z + \tfrac{3}{2})\hbar\omega\,\psi_{n_x n_y n_z}(\vec{r}) \\
&\equiv E_n\psi_{n_x n_y n_z},
\end{aligned}$$

for $n_x, n_y, n_z = 0, 1, 2, \ldots$

So the eigenfunctions are labelled by $n_x n_y n_z$ while the energy is given by their sum $n_x + n_y + n_z = n$

That is we need 3-independent integers n_x, n_y, n_z to label the independent eigenfunctions but only the sum fixes the energy of the eigenfunction, hence many eigenfunctions have the same energy

n	Energy	Eigenfunctions with Energy	Degeneracy
0	$\frac{3}{2}\hbar\omega$	ψ_{000}	1
1	$\frac{5}{2}\hbar\omega$	$\psi_{100}, \psi_{010}, \psi_{001}$	3
2	$\frac{7}{2}\hbar\omega$	$\psi_{200}, \psi_{020}, \psi_{002}, \psi_{110}, \psi_{101}, \psi_{011}$	6
3	$\frac{9}{2}\hbar\omega$	$\vdots$	$\vdots$
$\vdots$	$\vdots$		
n	$(n+\frac{3}{2})\hbar\omega$	ψ_{n00}	1
		$\psi_{n-1,1,0}$ $\psi_{n-1,0,1}$	2
		$\psi_{n-2,2,0}$ $\psi_{n-2,1,1}$ $\psi_{n-2,0,2}$	3
		$\vdots$	$\vdots$
		$\psi_{0,n,0}$ $\psi_{0,n-1,1}$ $\psi_{0,n-2,2} \cdots \psi_{0,0,n}$	$(n+1)$
$\vdots$		$\vdots$	

$$\sum_{m=1}^{n+1} m = \frac{(n+1)(n+2)}{2}$$

As required the degeneracy of the E_n eigenvalue is

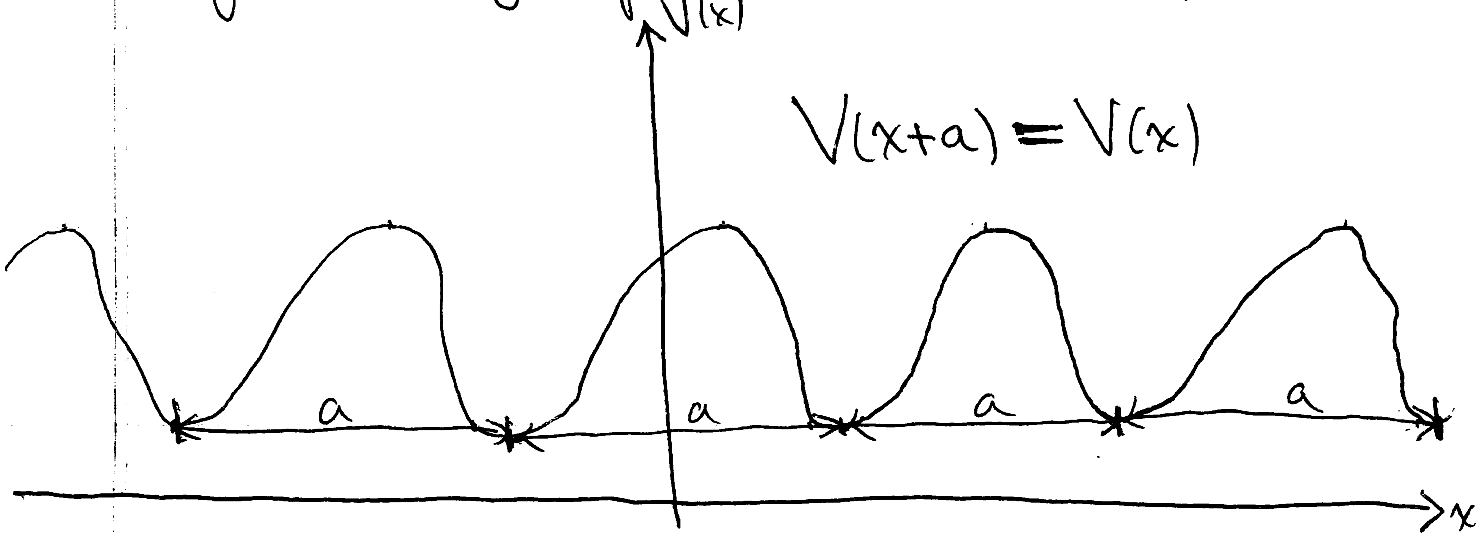
$$C^{n}_{n+3-1} = \frac{(n+3-1)!}{n!\,(3-1)!} = \frac{(n+2)(n+1)}{2}.$$

II. Applications In One-Dimension

2.2 Bound States

2.2.3. Periodic Potentials, Bloch's Theorem and the Kronig-Penny Model

A metal can be approximated by a set of positive ions forming a lattice with fixed sites while the valence electrons are conduction electrons moving subject to the lattice potential. This potential is periodic. For simplicity consider a 1-dimensional lattice and consider each electron to move separately under the influence of a periodic lattice potential



$$V(x+a) = V(x)$$

cell = period of length a.

Since this is an infinite array there is nothing to distinguish one cell from another. Hence the probability density and probability current density should also be periodic

1) $\rho(x+a) = \rho(x) \Rightarrow |\psi(x+a)|^2 = |\psi(x)|^2$

2) $S(x+a) = S(x) \Rightarrow \frac{\hbar}{2im}\left[\psi^*(x+a)\psi'(x+a) - \psi'^*(x+a)\psi(x+a)\right]$

$$= \frac{\hbar}{2im}\left[\psi^*(x)\psi'(x) - \psi'^*(x)\psi(x)\right]$$

Now 1) $\Rightarrow$ $\underline{\psi(x+a) = e^{i\varphi(x)}\psi(x)}$ with $\varphi(x) \in \mathbb{R}$.

Substituting into condition 2.)

$$S(x+a) = \frac{\hbar}{2im}\Big[\left(e^{i\varphi(x)}\psi(x)\right)^*\left(i\varphi'(x)e^{i\varphi(x)}\psi(x) + e^{i\varphi(x)}\psi'(x)\right)$$
$$- \left(i\varphi'(x)\psi(x)e^{i\varphi(x)} + e^{i\varphi(x)}\psi'(x)\right)^*\left(e^{i\varphi(x)}\psi(x)\right)\Big]$$

$$= \frac{\hbar}{2im}\left[\psi^*(x)\psi'(x) - \psi'^*(x)\psi(x) + 2i\varphi'(x)\psi^*(x)\psi(x)\right]$$

$$= S(x) + \frac{\hbar}{m}\frac{d\varphi(x)}{dx}|\psi(x)|^2$$

$$= S(x) \text{ by } (2.)$$

$\Rightarrow$ $\underline{\frac{\hbar}{m}\frac{d\varphi(x)}{dx}|\psi(x)|^2 = 0}$, thus $\frac{d\varphi(x)}{dx} = 0$

and $\varphi(x) = \varphi =$ constant independent of x.

Defining a constant q so that $\varphi \equiv q a$ we have

$$\underline{\psi(x+a) = e^{iqa}\psi(x) \quad \text{with } q \in \mathbb{R}.}$$

(see page -155'-)

For each choice of q we can label the wavefunction by q; $\psi_q(x)$, then we define the function $u_q(x)$ so that

$$\psi_q(x) \equiv e^{iqx} u_q(x).$$

Substituting this above, $\psi_q(x+a) = e^{iqa}\psi_q(x)$, which implies

$$e^{iq(x+a)} u_q(x+a) = e^{iqa} e^{iqx} u_q(x),$$

that is

$$u_q(x+a) = u_q(x),$$

$u_q(x)$ is a periodic function of x with period a. Thus we have

<u>Bloch's Theorem</u>: The wavefunction for a particle moving in a one-dimensional periodic potential can be written as

$$\psi_q(x) = e^{iqx} u_q(x)$$

with $u_q(x+a) = u_q(x)$, a being the period of the potential and $q \in \mathbb{R}$.

Note: In general we have that the Hamiltonian is invariant under translations in x by distance a. The translation operator is just the Taylor series operator; given any function $\psi(x)$

$$\psi(x+d) = \psi(x) + d\psi'(x) + \frac{d^2}{2!}\psi''(x) + \cdots + \frac{d^n}{n!}\psi^{(n)}(x) + \cdots$$

$$= e^{d\frac{d}{dx}}\psi(x), \quad \text{since } p = -i\hbar\frac{d}{dx}$$

$$= e^{\frac{i}{\hbar}pd}\psi(x) \equiv U(d)\psi(x)$$

$U(d)$ is the (unitary) translation operator through distance d. Now since $V(x) = V(x+a)$ we have for

$$H = \frac{p^2}{2m} + V(x)$$

$$[U(a), H] = \left[e^{\frac{i}{\hbar}pa}, \frac{p^2}{2m} + V(x)\right]$$

$$= \left[e^{a\frac{\partial}{\partial x}}, V(x)\right] = \left(V(x+a) - V(x)\right) \times e^{a\frac{\partial}{\partial x}}$$

$$= 0$$

Since $U(a)$ and H commute they can have common eigenfunctions. Thus

$$U(a)\,\psi(x) = \omega\,\psi(x)$$

$$H\,\psi(x) = E\,\psi(x).$$ Since U is unitary, i.e. p is Hermitian, the eigenvalues ω are just a phase factor, i.e. exponential of $i \times$ Real #. So

$$U(a)\psi(x) = e^{i\varphi}\psi(x), \quad \varphi \in \mathbb{R},$$

but

$$U(a)\psi(x) = \psi(x+a).$$ Hence we have $$\underline{\psi(x+a) = e^{i\varphi}\psi(x)\ ; \ \varphi \in \mathbb{R}.}$$

Note: it is sufficient to consider $-\pi < \varphi \leq \pi$ since $e^{i(\varphi+2\pi)} = e^{i\varphi}$, for

$\varphi = qa$, that it is sufficient to consider $-\frac{\pi}{a} < q \leq \frac{\pi}{a}$ in the first "Brillouin zone."

Above the lattice of sites was infinite and so we had no constraint on q other than it being real. Suppose instead the lattice is finite with length L which is some integer number of periods $L = Na$. If we impose periodic boundary conditions

$$\psi(x+L) = \psi(x) \quad , \; L = Na.$$

We have again the conditions of Bloch's Theorem but with only a denumerable set of q allowed. That is Bloch's Theorem implies

$$\begin{aligned}\psi_q(x+L) &= \psi_q(x+Na) \\ &= e^{iq(x+Na)}\, u_q(x) \\ &= e^{iqNa}\, \psi_q(x)\end{aligned}$$

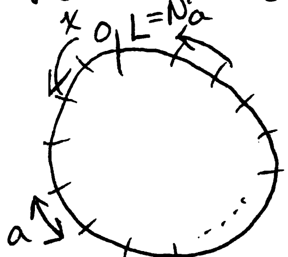
but by the periodic boundary condition this is just $\psi_q(x)$ hence

$$e^{iqNa} = 1$$

$$\Rightarrow \boxed{qa = \frac{2\pi m}{N}}$$

with $m = 0, \pm 1, \ldots, \pm\left(\frac{N}{2}-1\right), +\frac{N}{2}$

The sequence of allowed q values stops at $\frac{N}{2}=m$ since m higher than $\frac{N}{2}$ corresponds to translating by $qa > 2\pi$. Adding any multiple of 2π to qa does not change the physics, the state is the same. Specifically periodic boundary conditions identify $x=0$ with $x=L$; the x-axis becomes a circle (compact)



by increasing $x \to x+2\pi$

we just go around the circle to where we began. This cannot be a new state of the system, just a re-labelling of a previous state. To see this consider the state $\psi_q(x)$, we have

$$\psi_q(x+a) = e^{iqa}\psi_q(x),$$

shifting qa by 2π, that is letting $q \to q+\frac{2\pi}{a}$, is the same as letting $m \to m+N$. We then have

$$\psi_{q+\frac{2\pi}{a}}(x+a) = e^{i(q+\frac{2\pi}{a})a}\,\psi_{q+\frac{2\pi}{a}}(x)$$
$$= e^{iqa}\,\psi_{q+\frac{2\pi}{a}}(x).$$

But this is the same equation (i.e. same q)

that defines the state $\psi_q(x)$ i.e.

$$\psi_q(x+a) = e^{iqa}\psi_q(x). \text{ It is the } e^{iqa}$$

factor that delineates which state is being considered. Thus ψ_q and $\psi_{q+\frac{2\pi}{a}}$ describe the same state. Equivalently, shifting m by N brings us back to the same state. There are only N different m values

$$m = -\frac{N}{2}+1, \ldots, -1, 0, 1, 2, \ldots, +\frac{N}{2}-1, +\frac{N}{2}.$$

Choosing additional values of m just reproduces a state we have already counted with a lower m (q) label. Thus for a chain of periodic potentials with period a and chain length L=Na, the wavefunctions (energy eigenfunctions) have the form

$$\psi_q(x) = e^{iqx}u_q(x)$$

$$u_q(x+a) = u_q(x)$$

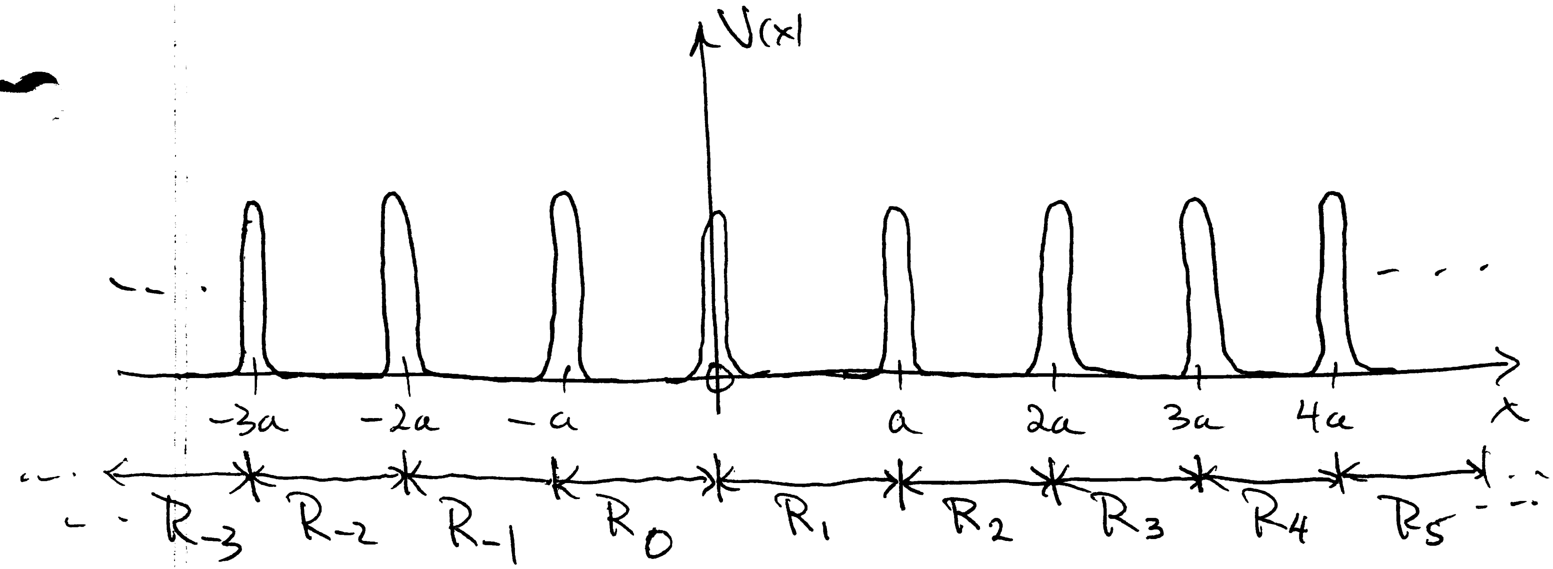
with $\quad q = \frac{2\pi}{a}\frac{m}{N}, \quad -\frac{N}{2}+1 \le m \le \frac{N}{2}$

m being an integer.

As an example of the application of Bloch's Theorem consider the case of an infinite chain of Dirac δ function potentials, the Kronig-Penny model. The potential of the model is defined as

$$V(x) = \frac{\hbar^2}{2m}\frac{\lambda}{a}\sum_{n=-\infty}^{+\infty}\delta(x-na)$$

with λ a real constant.



The x-axis is broken up into cells or regions R_n in which $(n-1)a < x < na$

(i.e. in region R_{n+1} x takes the values

$na < x < (n+1)a$)

With $E = \frac{\hbar^2 k^2}{2m}$, the Schrödinger equation is given by

$$-\frac{d^2}{dx^2}\psi(x) + \left[\frac{\lambda}{a}\sum_{n=-\infty}^{+\infty}\delta(x-na)\right]\psi(x) = k^2\psi(x).$$

Inside the regions, away from $x = na$, the potential vanishes and the Schrödinger equation becomes

$$\frac{d^2}{dx^2}\psi(x) + k^2\psi(x) = 0$$

which has the solution $\psi = A\sin kx + B\cos kx$.

So in each region R_n we label the wavefunction $\psi_{(n)}$.

For $x \in R_n$ it is given as $((n-1)a < x < na)$

$$\psi_{(n)}(x) = A_n \sin k(x-na) + B_n \cos k(x-na).$$

For $x \in R_{n+1}$ that is $na < x < (n+1)a$ the wavefunction has the form

$$\psi_{(n+1)}(x) = A_{n+1}\sin k(x-(n+1)a) + B_{n+1}\cos k(x-(n+1)a).$$

The boundary conditions for $\psi(x)$ can next be applied at $x = na$

The wavefunction must be continuous, hence

$$\psi(x=na^-) = \psi(x=na^+)$$

$$\Rightarrow \psi_{(n)}(na) = \psi_{(n+1)}(na)$$

$$\Rightarrow$$

1) $\boxed{B_n = -A_{n+1}\sin ka + B_{n+1}\cos ka}$

Since the potential is singular at $x=na$ we must integrate directly the Schrödinger equation to obtain the jump discontinuity in $\frac{d\psi}{dx}$ across $x=na$.

$$\int_{na-\epsilon}^{na+\epsilon} dx\left(\frac{d^2}{dx^2}\psi + k^2\psi\right) = \frac{\lambda}{a}\int_{na-\epsilon}^{na+\epsilon} dx \sum_{m=-\infty}^{+\infty} \delta(x-ma)\psi(x)$$

We now let $\epsilon \to 0^+$; since ψ is continuous

$$\lim_{\epsilon\to 0^+}\int_{na-\epsilon}^{na+\epsilon} dx\,\psi(x) = 0$$

while

$$\lim_{\epsilon\to 0^+}\int_{na-\epsilon}^{na+\epsilon} dx \frac{d}{dx}\left(\frac{d}{dx}\psi\right) = \frac{d}{dx}\psi\Big|_{x=na^+} - \frac{d}{dx}\psi\Big|_{x=na^-}$$

$$= \lim_{\epsilon\to 0^+}\frac{\lambda}{a}\int_{na-\epsilon}^{na+\epsilon} \delta(x-na)\psi(x) = \frac{\lambda}{a}\psi(na)$$

Thus we obtain the jump discontinuity in $\frac{d\psi}{dx}$

$$\frac{d}{dx}\psi\Big|_{x=na^+} - \frac{d}{dx}\psi\Big|_{x=na^-} = \frac{\lambda}{a}\psi(x=na)$$

$\Rightarrow$

2) $$\boxed{\begin{aligned} &+k\left[A_{n+1}\cos ka + B_{n+1}\sin ka\right] \\ &\quad -kA_n = \frac{\lambda}{a}B_n \end{aligned}}$$

Thus we have 2 equations which allow us to solve for A_{n+1}, B_{n+1} in terms of A_n, B_n

Multiply ① by $\sin ka$ and ② by $\frac{1}{k}\cos ka$ and subtract

$$B_n \sin ka - \frac{\lambda}{ka} B_n \cos ka - A_n \cos ka$$
$$= - A_{n+1} \sin^2 ka - A_{n+1} \cos^2 ka + \cancel{B_{n+1} \cos ka \sin ka} - \cancel{B_{n+1} \cos ka \times \sin ka}$$
$$= - A_{n+1}$$

$$\Rightarrow \boxed{A_{n+1} = A_n \cos ka + B_n\left[-\sin ka + \frac{\lambda}{ka}\cos ka\right]}$$

Multiply ① by $\cos ka$ and ② by $\frac{1}{k}\sin ka$ and add

$$B_n \cos ka + \frac{\lambda}{ka} B_n \sin ka + A_n \sin ka$$
$$= \cancel{-A_{n+1} \sin ka \cos ka} + B_{n+1} \cos^2 ka + \cancel{A_{n+1} \cos ka \sin ka} + B_{n+1} \sin^2 ka$$

B_{n+1}

Thus

$$\boxed{B_{n+1} = A_n \sin ka + B_n\left[\cos ka + \frac{\lambda}{ka}\sin ka\right]}$$

Finally we must impose the conditions of periodicity for the potential: Bloch's theorem

$$\psi(x+a) = e^{iqa}\psi(x).$$

For $x \in R_n$ we have

$$\psi_{(n)}(x) = A_n \sin k(x-na) + B_n \cos k(x-na),$$

when $x \in R_n$ this implies $x+a \in R_{n+1}$ and $\psi(x+a)$ is given by

$(x+a \in R_{n+1})$

$$\psi_{(n+1)}(x+a) = A_{n+1}\sin k(x+a-(n+1)a) + B_{n+1}\cos k(x+a-(n+1)a)$$

$$= A_{n+1}\sin k(x \quad na) + B_{n+} \cos k(x-na)$$

But Bloch's Theorem implies

$$\psi_{(n+1)}(x+a) = e^{iqa}\,\psi_{(n)}(x)$$

$$\Rightarrow \boxed{\begin{aligned} A_{n+1} &= e^{iqa} A_n \\ B_{n+1} &= e^{iqa} B_n \end{aligned}}$$

Substituting this into the boundary condition Relations for A_{n+1} and B_{n+1} we find

$$e^{iqa} A_n = A_n \cos ka + B_n\left[-\sin ka + \frac{\lambda}{ka}\cos ka\right]$$

$$e^{iqa} B_n = A_n \sin ka + B_n\left[\cos ka + \frac{\lambda}{ka}\sin ka\right]$$

$$\Rightarrow \boxed{\begin{bmatrix} e^{iqa} - \cos ka & \sin ka - \frac{\lambda}{ka}\cos ka \\ \sin ka & \cos ka + \frac{\lambda}{ka}\sin ka - e^{iqa} \end{bmatrix} \begin{bmatrix} A_n \\ B_n \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}}$$

Now if the matrix multiplying $\begin{bmatrix} A_n \\ B_n \end{bmatrix}$ has an inverse $A_n = B_n = 0$ which is the trivial solution and not physically relevant. Then the only way for a non-trivial solution to exist is for the determinant of the coefficient matrix to vanish i.e. the matrix has no inverse.

So

$$\left(e^{iqa} - \cos ka\right)\left(e^{iqa} - \cos ka - \frac{\lambda}{ka}\sin ka\right)$$

$$+ \sin ka\left(\sin ka - \frac{\lambda}{ka}\cos ka\right) = 0$$

$\Rightarrow$

$$0 = e^{2iqa} - e^{iqa}\left(2\cos ka + \frac{\lambda}{ka}\sin ka\right) + 1$$

multiply by e^{-iqa} $\Rightarrow$

$$0 = e^{iqa} + e^{-iqa} - \left(2\cos ka + \frac{\lambda}{ka}\sin ka\right)$$

or $2\cos qa = 2\cos ka + \frac{\lambda}{ka}\sin ka$

Then

$$\boxed{\cos qa = \cos ka + \frac{\lambda}{2}\frac{\sin ka}{ka}}$$

For a given q, this is a transcendental equation for ~~the~~ the eigenvalue k and hence $E = \frac{\hbar^2 k^2}{2m}$.

Defining $\theta \equiv ka$ so that

$$E = \frac{\hbar^2}{2ma^2}\theta^2,$$

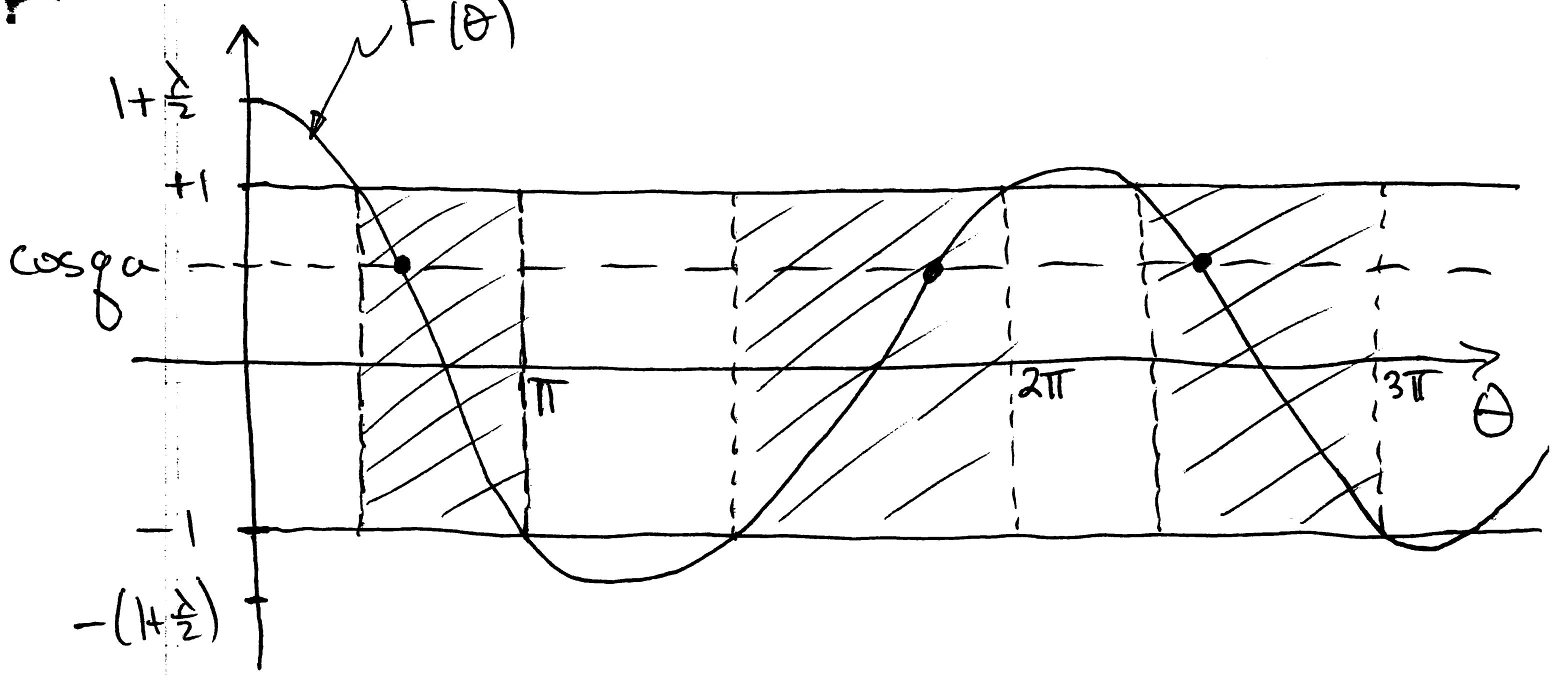
the transcendental equation becomes

$$\boxed{\begin{gathered}\cos qa = F(\theta)\\ \text{with } F(\theta) \equiv \cos\theta + \frac{\lambda}{2}\frac{\sin\theta}{\theta}.\end{gathered}}$$

As usual, we will solve this graphically.

$\cos qa$ is independent of θ with $|\cos qa| \leq 1$.

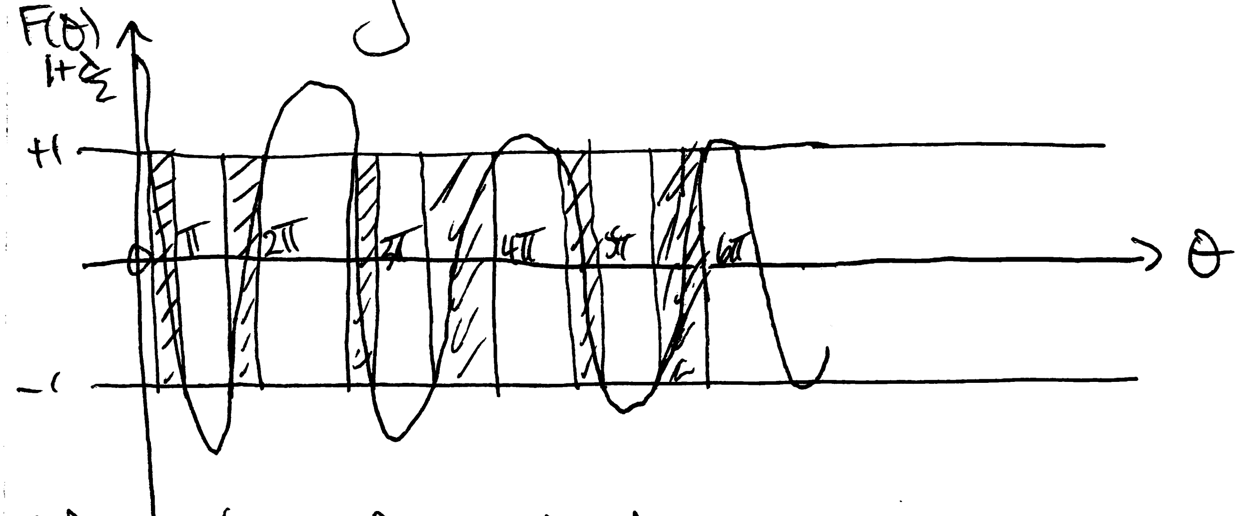
$F(\theta)$ is an oscillating function of θ with decreasing amplitude



Since $|\cos qa| \le 1$, solutions to the eigenvalue equation exist only for values of θ so that $|F(\theta)| \le 1$. These are the shaded regions above. Only certain discrete energy eigenvalues occur for a given q, indicated by the dots where the curves intersect. The allowed energy bands are separated by energy gaps when $|F(\theta)| > 1$. The width of the gap depends on the strength of the coupling λ. Even so, the left edge of each gap (or right edge of each band) can be found since it is where $F(\theta) = \pm 1$ and $\sin\theta = 0$ i.e. $\theta = n\pi$, $n = 1, 2, \ldots$

Finally consider the tight binding

approximation when the coupling $\lambda \to \infty$. Recall $F(\theta) = \cos\theta + \frac{\lambda}{2}\frac{\sin\theta}{\theta}$, and hence oscillates rapidly as λ grows. The allowed energy bands, values of θ where $|F(\theta)| \le 1$, become very narrow.



We still have that the right edge of each band is at $F(\theta) = \pm 1$ and $\sin\theta = 0$ i.e. $\theta = n\pi$, $n = 1, 2, \ldots$ As $\lambda \to \infty$ the band shrinks to just a point, the right edge $\theta = n\pi$. Hence as $\lambda \to \infty$ we have only the discrete energy eigenvalues given by

$$E_n = \frac{\hbar^2}{2ma^2}\theta_n^2 = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2$$

$$n = 1, 2, 3, \ldots$$