1. More on Bloch Functions. We showed in lecture that the wave function for the time independent Schroedinger equation with a periodic potential could be written as a Bloch function

$$e^{iqx}u_q(x) ,$$

where u_q is periodic with the same period as the potential.

(a) Show that u_q satisfies the differential equation

$$-\frac{\hbar^2}{2m}\frac{d^2u_q}{dx^2} - \frac{i\hbar^2 q}{m}\frac{du_q}{dx} + \frac{\hbar^2 q^2}{2m}u_q + Vu_q = Eu_q ,$$

where E is the energy.

Solution

We just plug the Bloch function into the Schroedinger equation:

$$\begin{aligned} Ee^{iqx}u_q &= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left(e^{iqx}u_q\right) + V(x)e^{iqx}u_q \\ &= -\frac{\hbar^2}{2m}\frac{d}{dx}\left(e^{iqx}\frac{du_q}{dx} + iqe^{iqx}u_q\right) + V(x)e^{iqx}u_q \\ &= -\frac{\hbar^2}{2m}\left(e^{iqx}\frac{d^2u_q}{dx^2} + iqe^{iqx}\frac{du_q}{dx} + iqe^{iqx}\frac{du_q}{dx} - q^2e^{iqx}u_q\right) + V(x)e^{iqx}u_q \\ &= -\frac{\hbar^2}{2m}\left(e^{iqx}\frac{d^2u_q}{dx^2} + 2iqe^{iqx}\frac{du_q}{dx} - q^2e^{iqx}u_q\right) + V(x)e^{iqx}u_q . \end{aligned}$$

After dividing out the traveling wave and some rearrangement, the desired result appears.

End Solution

(b) In fact, any wave 1D wave function can be written in the above form (with u_q not necessarily periodic) and will satisfy the above equation. The key point is that u_q is periodic with the same period ℓ as the potential. This means we only need to solve for u_q in an interval of length ℓ, $[0, \ell]$ or $[-a, a]$, say. ($2a = \ell$.) What are the boundary conditions on u_q at the ends of the interval? You should consider the case when V is well behaved at the ends of the interval.

Solution

u_q must be periodic with period ℓ. Therefore it must have the same value and the same derivative at both ends of the interval. Note that if we consider the periodic lattice of δ-functions, we have a problem if the δ-functions occur at the ends of the intervals. The problem can be avoided by shifting the interval to place the δ-functions somewhere else. Alternatively, if δ-functions occur at the ends of the intervals, then the boundary conditions are that u_q must have the same value at both ends of the interval and the difference in slopes u_q' must be given by the δ-function.

——— End Solution ———

(c) Solve u_q for the case of a periodic potential containing δ-function potential wells every $2a$ (the same case we did in lecture).

$$V(x) = -\lambda \sum_{n=-\infty}^{+\infty} \delta(x - a - n\ell) \, .$$

Since the u_q must be periodic, it doesn't matter where you place the interval of length ℓ. You might put it at $[0, \ell]$ so the potential well is in the middle of the interval.

——— Solution ———

The equation for u_q is a linear, homogeneous equation with constant coefficients. So, we should try a function like $\exp(ipx)$. Plugging this into the equation from part (a) gives (everywhere except at the δ-function in the potential),

$$\left(\frac{\hbar^2 p^2}{2m} + \frac{\hbar^2 pq}{m} + \frac{\hbar^2 q^2}{2m} \right) u_q = \frac{\hbar^2 k^2}{2m} \, u_q \, ,$$

where $k = \sqrt{2mE/\hbar^2}$. Simplifying,

$$(p+q)^2 = k^2 \, ,$$

or

$$p = -q \pm k \, .$$

If we put the δ-function at the middle of the interval, so the interval runs from $-a$ to $+a$ and the delta function is at 0, then the solution in the left half is

$$Ae^{i(-q+k)x} + Be^{i(-q-k)x} \, ,$$

and the solution in the right half is

$$Ce^{i(-q+k)x} + De^{i(-q-k)x} \, .$$

The continuity of u_q and its derivative at the ends of the interval gives

$$Ae^{i(+q-k)a} + Be^{i(+q+k)a} = Ce^{i(-q+k)a} + De^{i(-q-k)a}$$

$$i(-q+k)Ae^{i(+q-k)a} + i(-q-k)Be^{i(+q+k)a} = i(-q+k)Ce^{i(-q+k)a} + i(-q-k)De^{i(-q-k)a} \, .$$

A little algebra gives the solution for C and D in terms of A and B,

$$C = Ae^{i(+q-k)\ell} \, , \qquad D = Be^{i(+q+k)\ell} \, ,$$

with $\ell = 2a$. Next we need to satisfy the conditions at the location of the δ-function potential well at $x = 0$. Continuity of u_q gives

$$A + B = Ae^{i(+q-k)\ell} + Be^{i(+q+k)\ell} .$$

Setting the discontinuity of the slope equal to the integral of the delta function times $2m/\hbar^2$ gives

$$\begin{aligned} i(-q+k)Ae^{i(+q-k)\ell} + i(-q-k)Be^{i(+q+k)\ell} - i(-q+k)A - i(-q-k)B \\ = -2b(A+B) , \end{aligned}$$

where $b = m\lambda/\hbar^2$. These two equations can be rearranged

$$A\left(1 - e^{i(q-k)\ell}\right) + B\left(1 - e^{i(q+k)\ell}\right) = 0 ,$$

$$A\left(2b + i(q-k)\left(1 - e^{i(q-k)\ell}\right)\right) + B\left(2b + i(q+k)\left(1 - e^{i(q+k)\ell}\right)\right) = 0 .$$

We now have two homogeneous equations in two unknowns. These have non-trivial solutions only when the determinant of the matrix of coefficients vanishes. After a bit of algebra, one arrives at

$$\cos(ql) = \cos(kl) - \frac{b}{k}\sin(kl) ,$$

exactly the same expression for q we had when we solved the eigenvalue problem in lecture. There are solutions for real q as long as the right side is between -1 and $+1$. When it is outside this range, q will be imaginary and the Bloch function is not an acceptable solution. This will lead to energy gaps exactly as in lecture. Once q is known, the ratio B/A can be determined.

$$\frac{B}{A} = -\frac{1 - e^{i(q-k)\ell}}{1 - e^{i(q+k)\ell}} .$$

End Solution

2. The square well and the δ-function well. In lecture we discussed the energy levels in a square well $V = -V_0$ for $|x| < a$ and $V = 0$ for $|x| > a$. We also discussed the bound state of the δ-function potential well, $V = -\lambda\delta(x)$. Show that in the limit $V_0 \longrightarrow \infty$, $a \longrightarrow 0$, such that $2V_0 a \longrightarrow \lambda$, the ground state energy and the ground state wave function of the square well become the same as those for the δ-function well.

Solution

We found that the energies of the even states of the square well are given by solutions of the transcendental equation $q\tan(qa) = \kappa$ with $q = \sqrt{2m(V_0 + E)/\hbar^2}$ and $\kappa = \sqrt{-2mE/\hbar^2}$. Outside the well, the wave function is $\exp(-\kappa|x|)$. Considering the argument of the tangent, we note that as $a \longrightarrow 0$, $qa \longrightarrow 0$ since q contains the square root of

V_0. In the limit, then, $\kappa \longrightarrow q^2 a \longrightarrow 2mV_0 a/\hbar^2$. ($E$ inside the square root can be ignored since $V_0 \longrightarrow \infty$). Thus $\kappa \longrightarrow m\lambda/\hbar^2$. This is exactly what we found for the δ-function potential well with $\psi = \exp(-\kappa|x|)$ and ground state energy $-E = \hbar^2\kappa^2/2m = m\lambda^2/2\hbar^2$.

——— End Solution ———

3. The variational method. This is a subject I touched on in lecture but decided to save all the fun for the homework! Suppose you have a potential for which a ground state exists (the minimum energy of a stationary state is finite). You want to know the ground state energy but the potential is sufficiently complicated that you are unable to get an exact solution for the ground state wave function or the eigenvalue problem. The variational method consists in picking a "random" function which has at least one adjustable parameter, calculating the expectation value of the energy assuming the function you picked is the wave function of the system and then varying the parameter(s) to find the minimum energy. Of course, the function you pick must be square integrable (normalizable). Show that the minimum energy estimated this way has a lower bound which is the ground state energy. You may assume the spectrum is discrete.

——— Solution ———

With a discrete spectrum, we have energies E_n, $n = 0, 1, 2, \ldots$ where E_0 is the ground state energy and $E_0 \le E_n$ for all n. The trial wave function (assumed normalized) can be expanded in (orthonormal) stationary states.

$$\psi_{\text{trial}} = \sum_{n=0}^{\infty} c_n \psi_n \ ,$$

Then the expectation value of the energy in the state ψ_{trial} is

$$\begin{aligned} \langle E \rangle = \langle \psi_{\text{trial}} \mid H \mid \psi_{\text{trial}} \rangle &= \sum_{n=0}^{\infty} E_n |c_n|^2 \\ &\ge \sum_{n=0}^{\infty} E_0 |c_n|^2 = E_0 \sum_{n=0}^{\infty} |c_n|^2 = E_0 \ . \end{aligned}$$

——— End Solution ———

4. Variational method example. Use the variational method to estimate the ground state energy of the harmonic oscillator (with Hamiltonian $H = p^2/2m + m\omega^2 x^2/2$). We already know that the ground state wave function is a Gaussian, so **don't use a Gaussian trial wave function!** (That would be "cheating.") Pick some other simple function and see how close to $\hbar\omega/2$ you get. Note that if you pick a function with discontinuities (in the function or its derivative), you need to treat the discontinuities properly.

——— Solution ———

My trial function is a triangle. $\psi(x) = (1 - |x|/a)$ for $|x| < a$ and $\psi(x) = 0$ for $|x| > a$. The parameter is a. Note that it's even (the potential is even, so that's a good thing) and it's maximum where the potential well is deepest (which you would guess is the place the particle is most likely to be found). A bad thing about this trial function is that it has discontinuities in slope which (as we've seen) correspond to δ-functions in the potential and our potential is smooth.

To start, we calculate the normalization constant.

$$\langle \psi \mid \psi \rangle = 2 \int_0^a (1 - x/a)^2 \, dx = -\frac{2a}{3}(1 - x/a)^3 \bigg|_0^a = \frac{2a}{3} \, .$$

Next we calculate $\langle p^2/2m \rangle$ using the unnormalized ψ. Here we need to be a little careful because the p^2 involves a second derivative and the trial function has discontinuities in slope. We get around this by calculating $\langle p^\dagger \psi \mid p\psi \rangle$ rather than $\langle \psi \mid p^2 \psi \rangle$.

$$\begin{aligned}
\left\langle \frac{p^2}{2m} \right\rangle &= 2 \frac{1}{2m} \int_0^a \left(\frac{\hbar}{-i} \frac{d\psi^*}{dx} \right) \left(\frac{\hbar}{i} \frac{d\psi}{dx} \right) \\
&= \frac{2\hbar^2}{2m} \int_0^a \left(-\frac{1}{a} \right)^2 dx \\
&= \frac{\hbar^2}{ma} \, .
\end{aligned}$$

Now we calculate $\langle m\omega^2 x^2/2 \rangle$ (again with the unnormalized function).

$$\begin{aligned}
\left\langle \frac{1}{2} m\omega^2 x^2 \right\rangle &= m\omega^2 \int_0^a x^2 \left(1 - \frac{x}{a} \right)^2 dx \\
&= m\omega^2 \left(\frac{a^3}{3} - \frac{2a^3}{4} + \frac{a^3}{5} \right) \\
&= \frac{1}{30} m\omega^2 a^3 \, .
\end{aligned}$$

So, our the energy is (remembering to put in the normalization constant)

$$\langle E \rangle = \frac{3\hbar^2}{2ma^2} + \frac{m\omega^2 a^2}{20} \, .$$

We differentiate this with respect to a^2 and find that at the minimum energy, $a^2 = \sqrt{30}\hbar/m\omega$ and the minimum energy (for this function) is

$$\langle E \rangle_{\min} = \hbar\omega \left(\frac{3}{2\sqrt{30}} + \frac{\sqrt{30}}{20} \right) = \sqrt{\frac{3}{10}} \hbar\omega = \sqrt{\frac{6}{5}} \frac{1}{2} \hbar\omega = 1.095 \times \frac{1}{2} \hbar\omega \, .$$

Even with this crude function, the result is not bad!

End Solution

For additional fun (not to be turned in). What wold you do if you wanted to estimate E_1 as well as E_0 using the variational method?

5. "Bound states" in a periodic potential. In lecture we discussed the one-dimensional periodic potential made from delta functions,

$$V(x) = -\lambda \sum_{n=-\infty}^{+\infty} \delta(x - a - nl) ,$$

where $l = 2a$, so there are δ-functions at $(2n+1)a$ where n is any integer. In lecture we looked for energy eigenfunctions with energy $E > 0$. In this problem you are asked to find the energy eigenvalues with energy $E < 0$. These correspond to the bound state of the single delta function potential.

Solution

If $E < 0$, then define κ by

$$\frac{\hbar^2\kappa^2}{2m} = -E .$$

Then in the n^{th} interval, the solution is

$$\psi_n = A_n e^{\kappa x} + B_n e^{-\kappa x} ,$$

where A_n and B_n are constants to be determined later. We must join the solutions for each interval at the boundaries set by the δ-functions. ψ must be continuous:

$$A_{n+1}e^{-\kappa a} + B_{n+1}e^{\kappa a} = A_n e^{\kappa a} + B_n e^{-\kappa a} .$$

The derivative of the wave function must have a step given by the integral of the wave function times the potential:

$$\begin{aligned} \kappa A_{n+1}e^{-\kappa a} - \kappa B_{n+1}e^{\kappa a} - &\left(\kappa A_n e^{\kappa a} - \kappa B_n e^{-\kappa a}\right) \\ &= -\frac{2m\lambda}{\hbar^2}\frac{1}{2}\left(A_{n+1}e^{-\kappa a} + B_{n+1}e^{\kappa a} + A_n e^{\kappa a} + B_n e^{-\kappa a}\right) . \end{aligned}$$

Define $b = m\lambda/\hbar^2$. Then the two equations above can be summarized in matrix form as

$$\begin{pmatrix} e^{-\kappa a} & e^{\kappa a} \\ (\kappa + b)e^{-\kappa a} & (-\kappa + b)e^{\kappa a} \end{pmatrix} \begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = \begin{pmatrix} e^{\kappa a} & e^{-\kappa a} \\ (\kappa - b)e^{\kappa a} & (-\kappa - b)e^{-\kappa a} \end{pmatrix} \begin{pmatrix} A_n \\ B_n \end{pmatrix} .$$

The inverse of the left hand matrix above is

$$-\frac{1}{2\kappa}\begin{pmatrix} (-\kappa + b)e^{\kappa a} & -e^{\kappa a} \\ (-\kappa - b)e^{-\kappa a} & e^{-\kappa a} \end{pmatrix} .$$

Multiplying both sides of the above equation by this inverse yields

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = \begin{pmatrix} \left(1 - \frac{b}{k}\right) e^{\kappa l} & -\frac{b}{\kappa} \\ \frac{b}{\kappa} & \left(1 + \frac{b}{\kappa}\right) e^{-\kappa l} \end{pmatrix} \begin{pmatrix} A_n \\ B_n \end{pmatrix} = D \begin{pmatrix} A_n \\ B_n \end{pmatrix} .$$

Note that the matrix D has unit determinant so it has an inverse. Let the eigenvalues of D be d_1 and d_2. By the same argument we used in lecture, we only have a solution when $|d_1| = |d_2| = 1$ and $d_1 = d_2^*$.

We find the eignevalues from the characteristic equation:

$$\det \begin{pmatrix} \left(1 - \frac{b}{k}\right) e^{\kappa l} - d & -\frac{b}{\kappa} \\ \frac{b}{\kappa} & \left(1 + \frac{b}{\kappa}\right) e^{-\kappa l} - d \end{pmatrix} = 0 \,,$$

or

$$d^2 - 2d \left(\cosh(\kappa l) - \frac{b}{\kappa} \sinh(\kappa l) \right) + 1 = 0 \,.$$

Solutions for the eigenvalues are:

$$d = \xi \pm \sqrt{\xi^2 - 1} \,, \qquad \xi = \cosh(\kappa l) - \frac{bl}{\kappa l} \sinh(\kappa l) \,.$$

In order that $|d| = 1$, we must have $-1 < \xi < +1$. So the next step is to decide for what values of bl and κl we can meet this condition. A good way to find out is to use excel or matlab to generate various plots. However, the following things can be said. First of all, $\cosh(0) = 1$ and $\sinh(0) = 0$ and $\sinh(x) < \cosh(x)$ for all x. For large x, $\cosh(x) \to \exp(x)/2$, $\sinh(x) \to \exp(x)/2$ and the difference between the two is $\exp(-x)$ (for all x). As $x \to 0$, $\sinh(x)/x \to 1$.

So, if $bl = 0$ (that is, no potential), there is no solution. This is to be expected. If $bl > 0$ there are always solutions and a single band of energies for which solutions exist. If $bl < 2$, the band extends up to $E = 0$. If $bl > 2$, a zero energy solution does not exist and the band is below zero. For very large bl, the band will be a narrow range with $\kappa l \approx bl$ (since $\cosh(\kappa l) \approx \sinh(\kappa l)$ for large κl). Note that for a single delta function, the solution was $\kappa = b$, so when the potential is large, the bound state from a single δ-function does not reach the adjacent δ-functions and there is little change to the energy of the bound state leading to a relatively narrow band of energies. On the other hand, when $bl \lesssim 1$, the bound state wave functions do overlap the adjacent δ-functions, so there are significant changes to the energies leading to a relatively broad band of energies.

You weren't asked to find the energy eigenfunctions. However, it is interesting to note that since $|d| = 1$ for a solution, we can write $d_\pm = \exp(\pm iql)$ and generate the eigenfunctions just as we did for the positive energy solutions. So, we will find traveling wave solutions even in this case!

— End Solution —