Problem Set 10 **Solutions**
8.04 Spring 2013 **Thursday, May 9**

Problem 1. (5 points) Zero Point Energy in a Lattice

Requiring $g_o \gg 1$ means that the barriers are very strong. In this case, transmission across the barriers is very small so the electrons can be approximated as mostly trapped inside individual wells. We can thus estimate the ground state energy by using the formula for the ground state of an infinite well of length L,

$$E_{g.s.} = \frac{\pi^2 \hbar^2}{2mL^2}, \tag{1}$$

On the other hand, if the barriers were weak ($g_o \ll 1$), the electrons would essentially be free to roam the entire crystal of length D, and the zero point energy would be given by

$$E_{g.s.} = \frac{\pi^2 \hbar^2}{2mD^2}. \tag{2}$$

which is much lower than the value in Equation 1, since $D \gg L$.

This explains an important property of solids: as long as you are looking at chunks of the solid that are parametrically larger than the inter-atomic spacing ($D \gg L$), the basic material properties of the solid (opacity, conductivity, etc) do not change as you study larger and larger chunks. Note that this would not be true in the absence of the periodic lattice!

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Problem 2. (5 points) Blinded by Science

A material is opaque to light of frequency f if it efficiently absorbs photons of $E = hf$. To do so while conserving energy, the material must be able to move from its initial state to an excited state whose energy differs by $E_f - E_i = hf$.

Suppose we fire a photon of frequency f at a Diamond. To absorb the photon, one of the electrons in the (filled) valence band must be excited into an unoccupied excited state. But the first available excited state is E_{gap} above the highest-energy available electron! So it is simply impossible for the diamond to absorb the photon unless $hf \geq E_{gap}$. Photons with energy less than E_{gap} simply cannot be absorbed by the diamond. Diamonds are thus *transparent* to photons with frequencies lower than

$$f_{min} = \frac{E_{gap}}{h} \sim 1.3 \times 10^{15}\,\text{Hz} \ . \tag{3}$$

This minimum frequency corresponds to a maximum wavelength of 230 nanometers, which is well into the ultraviolet band. Above this frequency (or below this wavelength) photons can be absorbed, and diamond is opaque – but since the human eye is sensitive only to light in the wavelength range of $\sim 400 - 700\,\text{nm}$, diamonds appear translucent[1].

So why would a diamond ever be anything other than perfectly clear? For a particular diamond to absorb visible light with $hf < E_{gap}$, there must be some extra states inside the bandgap. This implies that the periodic-crystal approximation was not accurate. For example, there may be impurities in the lattice, eg points in the lattice where a carbon atom is replaced by another atom with a different number of valence electrons. In the case of blue diamonds, this is typically due to a dust of boron atoms, each of which has one less valence electron than the carbon it has displaced.

[1] Of course, photons *can* Bragg-scatter off the diamond lattice, hence the spectacular dance of light that scatters off my wife's engagement ring when she waves her hand in the sunlight.

Problem Set 10 **Solutions**
8.04 Spring 2013 **Thursday, May 9**

Problem 3. (5 points) The World is Full of Fermions...

To determine whether hydrogen atoms are bosons or fermions it suffices to take two hydrogen atoms and swap them. If the wavefunction changes sign under this exchange operation, the atoms are fermions; if not, they are bosons. Now, since each Hydrogen atom is a bound state of an electron and a proton, the wavefunction for two hydrogen atoms takes the form,

$$\psi(H_1, H_2) \equiv \psi(\underbrace{e_1, p_1}_{\text{1st atom}}\,;\,\underbrace{e_2, p_2}_{\text{2nd atom}}), \tag{4}$$

where e_1 represents the coordinates and the spin of the electron belonging to the first atom, p_2 those of the second proton, and so forth. We want to know what happens to the wavefunction as we exchange H_1 and H_2,

$$\psi(H_1, H_2) = \pm_? \, \psi(H_2, H_1) \tag{5}$$

To exchange the two atoms, we can simply exchange the constituent electrons and protons. But the electrons are ferions, and the protons are fermions, so exchanging them in pairs we find,

$$\psi(e_1, p_1; e_2, p_2) \overset{e_1 \rightleftarrows e_2}{=} (-1)\,\psi(e_2, p_1; e_1, p_2) \overset{p_1 \rightleftarrows p_2}{=} (-1)^2 \psi(e_2, p_2; e_1, p_1) \tag{6}$$

so

$$\psi(H_1, H_2) = +\,\psi(H_2, H_1) \tag{7}$$

i.e. Hydrogen atoms are bosons.

The same logic applies to bound states of N fermions: for each pair of constituent fermions exchanged, the wavefunctions acquires a minus sign; when we are done with exchanging all N constituent fermions between the two bound states, the wavefunction will have acquired a factor of $(-1)^N$. Thus bound states of N fermions are bosons if N is even (the wavefunction is even under the exchange of two such bound states) and fermions if N is odd (the wavefunction changes sign under exchange)

Note: In quantum field theory there is a theorem (the spin-statistics theorem) which states that all half-integer spin particles are fermions and all integer spin particles are bosons. This theorem can be used to construct an alternate proof. The total spin of the composite system of a proton and an electron is the vectorial sum of the individual spins:

$$\vec{S}_H = \vec{S}_p + \vec{S}_e, \tag{8}$$

from which follows that a measurement of the total spin along an arbitrary direction $\hat{n}$:

$$\hat{n} \cdot \vec{S}_H = \hat{n} \cdot \vec{S}_p + \hat{n} \cdot \vec{S}_e \tag{9}$$

can have only the results:

$$\hat{n} \cdot \vec{S}_H : \left\{ \frac{1}{2} + \frac{1}{2}, \frac{1}{2} - \frac{1}{2}, -\frac{1}{2} + \frac{1}{2}, -\frac{1}{2} - \frac{1}{2} \right\} = \{1, 0, 0, -1\}. \tag{10}$$

We see that all possible eigenvalues are integers, so the hydrogen atom is a boson.

Generally for an arbitrary number N of fermions the possible eigenvalues for the total spin have the form:

$$\sum_{i=1}^{N} \frac{2m_i + 1}{2} = \underbrace{\sum_{i=1}^{N} m_i}_{integer} + \frac{1}{2}N = \begin{cases} half - integer & N\ odd \\ integer & N\ even \end{cases}, \tag{11}$$

where m_i's are integers.

Problem 4. (20 points) Identical Particles and Spooky Correlations

(a) **(3 points)** This is just a simple matter of calculating the expectation values for x_1 and x_2:

$$\begin{aligned}\langle x_1 \rangle_D &= \int_{-\infty}^{-\infty}\int_{-\infty}^{-\infty} \psi_D(x_1,x_2)^* x_1 \psi_D(x_1,x_2)\, dx_1 dx_2 \\ &= \int_{-\infty}^{-\infty} \phi_0(x_1)^* x_1 \phi_0(x_1)\, dx_1 \times \underbrace{\int_{-\infty}^{-\infty} \phi_1(x_2)^* \phi_1(x_2)\, dx_2}_{=1} \\ &= \frac{1}{\rho\sqrt{\pi}} \int_{-\infty}^{-\infty} x_1 e^{-{x_1}^2/\rho^2} dx_1 = 0 \end{aligned} \tag{12}$$

$$\begin{aligned}\langle x_2 \rangle_D &= \int_{-\infty}^{-\infty}\int_{-\infty}^{-\infty} \psi_D(x_1,x_2)^* x_2 \psi_D(x_1,x_2)\, dx_1 dx_2 \\ &= \underbrace{\int_{-\infty}^{-\infty} \phi_0(x_1)^* \phi_0(x_1)\, dx_1}_{=1} \times \int_{-\infty}^{-\infty} \phi_1(x_2)^* x_2 \phi_1(x_2)\, dx_2 \\ &= \frac{2}{\rho\sqrt{\pi}} \int_{-\infty}^{-\infty} \frac{{x_2}^3}{\rho^2} e^{-{x_2}^2/\rho^2} dx_2 = 0, \end{aligned} \tag{13}$$

where we used the fact that the final integrands are odd functions.

$$
\begin{aligned}
\langle x_1 \rangle_{S/A} \quad &= \int_{-\infty}^{-\infty} \int_{-\infty}^{-\infty} \psi_{S/A}\left(x_1, x_2\right)^* x_1 \psi_{S/A}\left(x_1, x_2\right) dx_1 dx_2 \\
&= \frac{1}{2} \underbrace{\int_{-\infty}^{-\infty} \phi_0\left(x_1\right)^* x_1 \phi_0\left(x_1\right) dx_1 \times \int_{-\infty}^{-\infty} \phi_1\left(x_2\right)^* \phi_1\left(x_2\right) dx_2}_{=\langle x_1 \rangle_D = 0} \\
&\pm \frac{1}{2} \int_{-\infty}^{-\infty} \phi_0\left(x_1\right)^* x_1 \phi_1\left(x_1\right) dx_1 \times \underbrace{\int_{-\infty}^{-\infty} \phi_1\left(x_2\right)^* \phi_0\left(x_2\right) dx_2}_{=0} \\
&\pm \frac{1}{2} \int_{-\infty}^{-\infty} \phi_1\left(x_1\right)^* x_1 \phi_0\left(x_1\right) dx_1 \times \underbrace{\int_{-\infty}^{-\infty} \phi_0\left(x_2\right)^* \phi_1\left(x_2\right) dx_2}_{=0} \\
&+ \frac{1}{2} \underbrace{\int_{-\infty}^{-\infty} \phi_1\left(x_1\right)^* x_1 \phi_1\left(x_1\right) dx_1 \times \int_{-\infty}^{-\infty} \phi_0\left(x_2\right)^* \phi_0\left(x_2\right) dx_2}_{x_1 \rightleftarrows x_2 \Rightarrow = \langle x_2 \rangle_D = 0} = 0 \quad (14)
\end{aligned}
$$

$$
\begin{aligned}
\langle x_2 \rangle_{S/A} \quad &= \int_{-\infty}^{-\infty} \int_{-\infty}^{-\infty} \psi_{S/A}\left(x_1, x_2\right)^* x_2 \psi_{S/A}\left(x_1, x_2\right) dx_1 dx_2 \\
&= \frac{1}{2} \underbrace{\int_{-\infty}^{-\infty} \phi_0\left(x_1\right)^* \phi_0\left(x_1\right) dx_1 \times \int_{-\infty}^{-\infty} \phi_1\left(x_2\right)^* x_2 \phi_1\left(x_2\right) dx_2}_{=\langle x_2 \rangle_D = 0} \\
&\pm \frac{1}{2} \underbrace{\int_{-\infty}^{-\infty} \phi_0\left(x_1\right)^* \phi_1\left(x_1\right) dx_1}_{=0} \times \int_{-\infty}^{-\infty} \phi_1\left(x_2\right)^* x_2 \phi_0\left(x_2\right) dx_2 \\
&\pm \frac{1}{2} \underbrace{\int_{-\infty}^{-\infty} \phi_1\left(x_1\right)^* \phi_0\left(x_1\right) dx_1}_{=0} \times \int_{-\infty}^{-\infty} \phi_0\left(x_2\right)^* x_2 \phi_1\left(x_2\right) dx_2 \\
&+ \frac{1}{2} \underbrace{\int_{-\infty}^{-\infty} \phi_1\left(x_1\right)^* \phi_1\left(x_1\right) dx_1 \times \int_{-\infty}^{-\infty} \phi_0\left(x_2\right)^* x_2 \phi_0\left(x_2\right) dx_2}_{x_1 \rightleftarrows x_2 \Rightarrow = \langle x_1 \rangle_D = 0} = 0. \quad (15)
\end{aligned}
$$

Another way to compute $\langle x_2 \rangle_{S/A}$ is to make use of the symmetry properties of $\psi_{S/A}\left(x_1, x_2\right)$. Let's consider some function $f(x_2)$ and compute its expectation value:

$$\begin{aligned}
\langle f(x_2)\rangle_{S/A} &= \int_{-\infty}^{-\infty}\int_{-\infty}^{-\infty} \psi_{S/A}(x_1,x_2)^* f(x_2)\,\psi_{S/A}(x_1,x_2)\,dx_1dx_2 \\
&\overset{x_1\rightleftarrows x_2}{=} \int_{-\infty}^{-\infty}\int_{-\infty}^{-\infty} \psi_{S/A}(x_2,x_1)^* f(x_1)\,\psi_{S/A}(x_2,x_1)\,dx_2dx_1 \\
&= \int_{-\infty}^{-\infty}\int_{-\infty}^{-\infty} \left[\pm\psi_{S/A}(x_1,x_2)^*\right] f(x_1)\left[\pm\psi_{S/A}(x_1,x_2)\right] dx_2dx_1 \\
&= \int_{-\infty}^{-\infty}\int_{-\infty}^{-\infty} \psi_{S/A}(x_1,x_2)^* f(x_1)\,\psi_{S/A}(x_1,x_2)\,dx_2dx_1 \\
&= \langle f(x_1)\rangle_{S/A}\,. \qquad (16)
\end{aligned}$$

(b) **(4 points)** In order to compute $\langle (x_1-x_2)^2\rangle = \langle {x_1}^2\rangle - 2\langle x_1x_2\rangle + \langle {x_2}^2\rangle$, for each wavefunction we have to calculate three expectation values: $\langle {x_1}^2\rangle$, $\langle {x_2}^2\rangle$, and $\langle x_1x_2\rangle$.

ψ_D:

$$\begin{aligned}
\left\langle {x_1}^2\right\rangle_D &= \int_{-\infty}^{-\infty}\int_{-\infty}^{-\infty} \psi_D(x_1,x_2)^* {x_1}^2 \psi_D(x_1,x_2)\,dx_1dx_2 \\
&= \int_{-\infty}^{-\infty} \phi_0(x_1)^* {x_1}^2 \phi_0(x_1)\,dx_1 \times \underbrace{\int_{-\infty}^{-\infty} \phi_1(x_2)^*\phi_1(x_2)\,dx_2}_{=1} \\
&= \frac{1}{\rho\sqrt{\pi}}\int_{-\infty}^{-\infty} {x_1}^2 e^{-{x_1}^2/\rho^2} dx_1 = \frac{\rho^2}{2} \qquad (17)
\end{aligned}$$

$$\begin{aligned}
\left\langle {x_2}^2\right\rangle_D &= \int_{-\infty}^{-\infty}\int_{-\infty}^{-\infty} \psi_D(x_1,x_2)^* {x_2}^2 \psi_D(x_1,x_2)\,dx_1dx_2 \\
&= \underbrace{\int_{-\infty}^{-\infty} \phi_0(x_1)^*\phi_0(x_1)\,dx_1}_{=1} \times \int_{-\infty}^{-\infty} \phi_1(x_2)^* {x_2}^2 \phi_1(x_2)\,dx_2 \\
&= \frac{2}{\rho\sqrt{\pi}}\int_{-\infty}^{-\infty} \frac{{x_2}^4}{\rho^2} e^{-{x_2}^2/\rho^2} dx_2 = \frac{3\rho^2}{2} \qquad (18)
\end{aligned}$$

$$\begin{aligned}
\langle x_1x_2\rangle_D &= \int_{-\infty}^{-\infty}\int_{-\infty}^{-\infty} \psi_D(x_1,x_2)^* x_1x_2 \psi_D(x_1,x_2)\,dx_1dx_2 \\
&= \underbrace{\int_{-\infty}^{-\infty} \phi_0(x_1)^* x_1 \phi_0(x_1)\,dx_1}_{=\langle x_1\rangle_D=0} \times \underbrace{\int_{-\infty}^{-\infty} \phi_1(x_2)^* x_2 \phi_1(x_2)\,dx_2}_{=\langle x_2\rangle_D=0} = 0 \qquad (19)
\end{aligned}$$

and

$$\left\langle (x_1-x_2)^2\right\rangle_D = \frac{\rho^2}{2} + \frac{3\rho^2}{2} - 0 = 2\rho^2. \qquad (20)$$

$\psi_{S/A}$:

$$\begin{aligned}
\left\langle {x_1}^2 \right\rangle_{S/A} = \left\langle {x_2}^2 \right\rangle_{S/A} \quad &= \int_{-\infty}^{-\infty}\int_{-\infty}^{-\infty} \psi_{S/A}\left(x_1,x_2\right)^* {x_1}^2 \psi_{S/A}\left(x_1,x_2\right) dx_1 dx_2 \\
&= \frac{1}{2}\underbrace{\int_{-\infty}^{-\infty} \phi_0\left(x_1\right)^* {x_1}^2 \phi_0\left(x_1\right) dx_1 \times \int_{-\infty}^{-\infty} \phi_1\left(x_2\right)^* \phi_1\left(x_2\right) dx_2}_{=\langle {x_1}^2\rangle_D = \frac{\rho^2}{2}} \\
&\pm\frac{1}{2}\int_{-\infty}^{-\infty} \phi_0\left(x_1\right)^* {x_1}^2 \phi_1\left(x_1\right) dx_1 \times \underbrace{\int_{-\infty}^{-\infty} \phi_1\left(x_2\right)^* \phi_0\left(x_2\right) dx_2}_{=0} \\
&\pm\frac{1}{2}\int_{-\infty}^{-\infty} \phi_1\left(x_1\right)^* {x_1}^2 \phi_0\left(x_1\right) dx_1 \times \underbrace{\int_{-\infty}^{-\infty} \phi_0\left(x_2\right)^* \phi_1\left(x_2\right) dx_2}_{=0} \\
&+\frac{1}{2}\underbrace{\int_{-\infty}^{-\infty} \phi_1\left(x_1\right)^* {x_1}^2 \phi_1\left(x_1\right) dx_1 \times \int_{-\infty}^{-\infty} \phi_0\left(x_2\right)^* \phi_0\left(x_2\right) dx_2}_{x_1 \rightleftarrows x_2 \Rightarrow = \langle {x_2}^2\rangle_D = \frac{3\rho^2}{2}} \\
&= \rho^2
\end{aligned} \tag{21}$$

$$\begin{aligned}
\left\langle x_1 x_2 \right\rangle_{S/A} \quad &= \int_{-\infty}^{-\infty}\int_{-\infty}^{-\infty} \psi_{S/A}\left(x_1,x_2\right)^* x_1 x_2 \psi_{S/A}\left(x_1,x_2\right) dx_1 dx_2 \\
&= \frac{1}{2}\underbrace{\int_{-\infty}^{-\infty} \phi_0\left(x_1\right)^* x_1 \phi_0\left(x_1\right) dx_1}_{=\langle x_1\rangle_D = 0} \times \underbrace{\int_{-\infty}^{-\infty} \phi_1\left(x_2\right)^* x_2 \phi_1\left(x_2\right) dx_2}_{=\langle x_2\rangle_D = 0} \\
&\pm\frac{1}{2}\int_{-\infty}^{-\infty} \phi_0\left(x_1\right)^* x_1 \phi_1\left(x_1\right) dx_1 \times \int_{-\infty}^{-\infty} \phi_1\left(x_2\right)^* x_2 \phi_0\left(x_2\right) dx_2 \\
&\pm\frac{1}{2}\int_{-\infty}^{-\infty} \phi_1\left(x_1\right)^* x_1 \phi_0\left(x_1\right) dx_1 \times \int_{-\infty}^{-\infty} \phi_0\left(x_2\right)^* x_2 \phi_1\left(x_2\right) dx_2 \\
&+\frac{1}{2}\underbrace{\int_{-\infty}^{-\infty} \phi_1\left(x_1\right)^* x_1 \phi_1\left(x_1\right) dx_1}_{x_1 \rightleftarrows x_2 \Rightarrow = \langle x_2\rangle_D = 0} \times \underbrace{\int_{-\infty}^{-\infty} \phi_0\left(x_2\right)^* x_2 \phi_0\left(x_2\right) dx_2}_{x_1 \rightleftarrows x_2 \Rightarrow = \langle x_1\rangle_D = 0} \\
&= \pm\left(\int_{-\infty}^{-\infty} \phi_0\left(x_1\right)^* x_1 \phi_1\left(x_1\right) dx_1\right)^2 \\
&= \pm\left(\frac{\sqrt{2}}{\rho\sqrt{\pi}}\int_{-\infty}^{-\infty} \frac{{x_1}^2}{\rho} e^{-{x_1}^2/\rho^2} dx_1\right)^2 = \pm\left(\frac{\rho}{\sqrt{2}}\right)^2 \\
&= \pm\frac{\rho^2}{2}
\end{aligned} \tag{22}$$

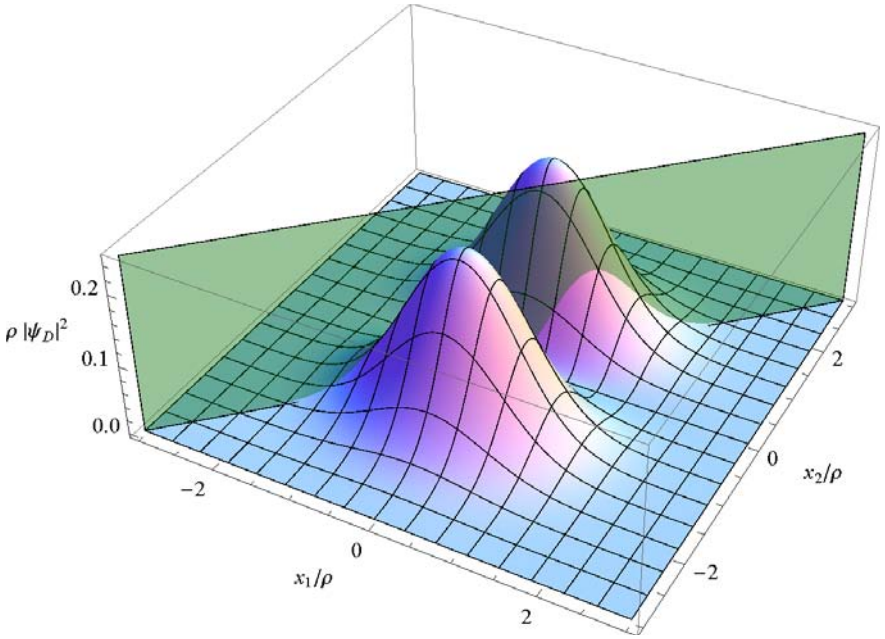
and

$$\left\langle (x_1 - x_2)^{\,2} \right\rangle_{S/A} = \rho^2 + \rho^2 - 2\left(\pm\frac{\rho^2}{2}\right) = \begin{cases} \rho^2 & S \\ 3\rho^2 & A \end{cases}. \tag{23}$$

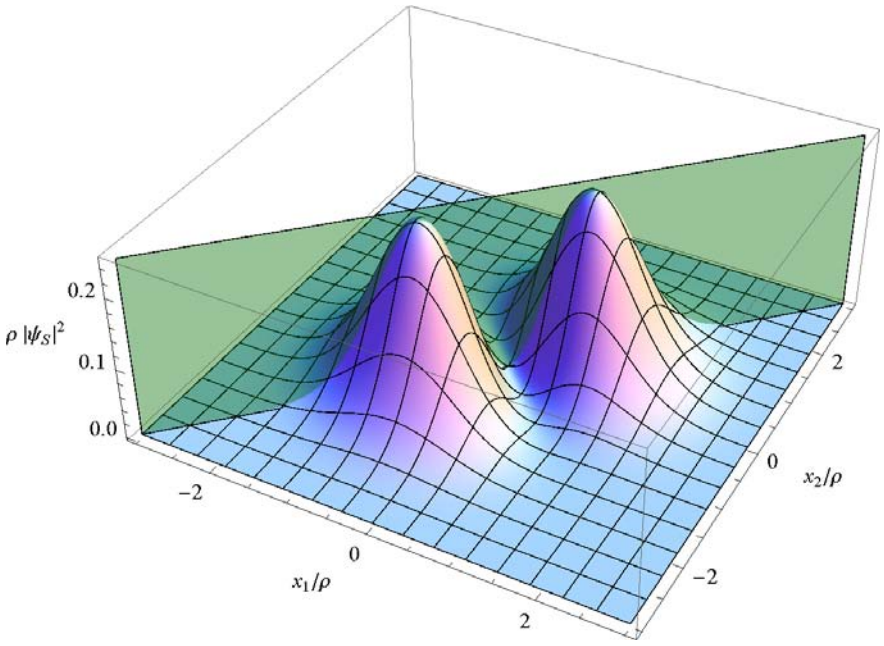
We see that the mean separation between particles is the smallest for the symmetric wavefunction and the biggest for the antisymmetric wavefunction. This means that in the bosonic case the two particles are more likely to stay close together than in the fermionic case, and the case of distinguishable particles is in the middle. The two particles do not experience different forces. However, we can interpret the values of the mean square distances as an effective attraction/repulsion between the two particles. This is due to the symmetry properties of the corresponding wavefunctions. For example, the antisymmetric wavefunction is such that $\psi_A(x_1, x_1) = 0$, i.e. the two particles will *never* be at the same place, and it is intuitive to think of this as an effective repulsion. Note instead that $\psi_S(x_1, x_1) = \sqrt{2}\psi_D(x_1, x_1)$, which means that when the wavefunction is symmetric the two particles are *more* likely to be at the same place than in the distinguishable case, hence we can interpret this as an effective attraction between the two bosons.

(c) **(3 points)** Below are shown the probability densities associated with the three wavefunctions (units indicated on the figures). The semi-transparent green rectangle represent the $x_1 = x_2$ plane.

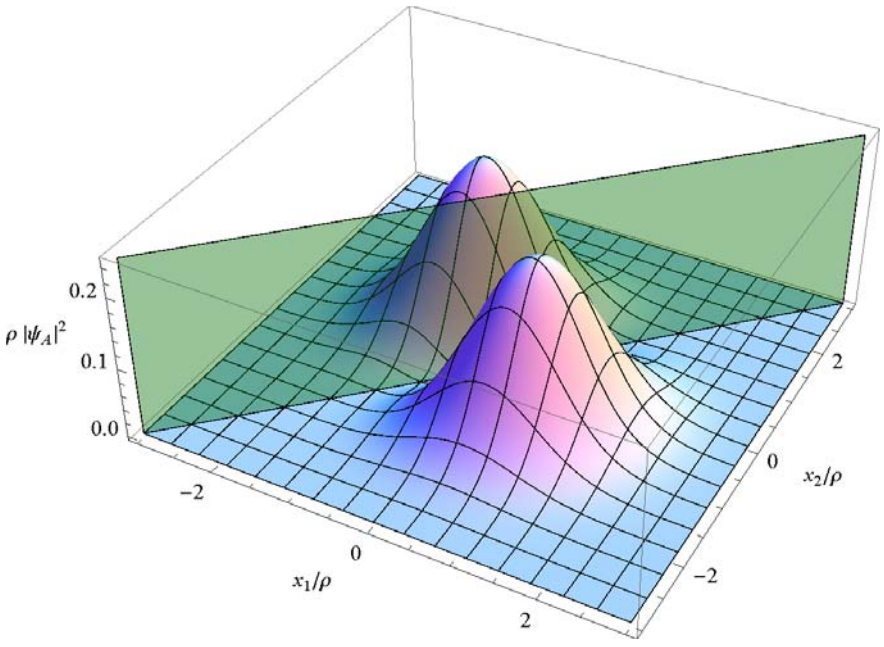
ψ_D:



ψ_S:



ψ_A:



Again we see that for $x_1 = x_2$ the probability density is maximal for the symmetric wavefunction and minimal (actually null) for the antisymmetric wavefunction.

(d) **(5 points)** By assumption, the N particles we place in the trap do not interact with each other, so the N-particle energy operator $\hat{\mathcal{E}}$ takes the simple form,

$$\hat{\mathcal{E}} = \sum_{i=1}^{N} \hat{E}_i$$

The system is thus separable, with N-particle energy eigenstates and energies

$$\Psi_{n_1,\ldots n_N}(x_1,\ldots,x_N) = \varphi_{n_1}(x_1)\ldots\varphi_{n_N}(x_N)\,, \qquad \mathcal{E}_{\{n_i\}} = \sum_{i=1}^{N} E_{n_i}$$

with $\varphi_n(x)$ and E_n being the single-particle energy eigenstates and eigenenergies. The lowest possible energy for N particles is thus $E^N_{min} = N\,E_1$ corresponding to all particles being in the single-particle ground state,

$$\Psi_{\{1,\ldots,1\}}(x_1,\ldots,x_N) = \varphi_1(x_1)\ldots\varphi_1(x_N)\,, \qquad \mathcal{E}_{min} = N\,E_1$$

If the N particles in our box are identical bosons, it is possible to put them all in the same state, and in particular it is possible to put them in the same single-particle ground state as above. The N-boson ground state Ψ^B_1 is thus

$$\Psi^B_1(x_1,\ldots,x_N) = \varphi_1(x_1)\varphi_1(x_2)\cdots\varphi_1(x_N), \qquad \mathcal{E}^B_1 = N\,E_1$$

which is invariant under the exchange of any pair of particles, as is required for the wavefunction to describe identical bosons, as one can easily check.

The first excited level, Ψ^B_2, is then obtained by raising a single particle to the next allowed single-particle eigenstate. However, the wavefunction for N bosons must be completely symmetric under the interchange of any two bosons, so the amplitude to raise any one of the N bosons must be equal, giving

$$\Psi^B_2(x_1,\ldots,x_N) = C^B \sum_{i=1}^{N} \Psi^B_1(x_1,\ldots,x_{i-1},x_{i+1},\ldots,x_N)\varphi_2(x_i), \quad \mathcal{E}^B_2 = (N-1)\,E_1 + E_2\,.$$

By construction, Ψ^B_2 is symmetric under any permutation $\mathcal{P}_{ij}$. The minimum energy required to excite the system of N bosons is thus simply

$$\Delta\mathcal{E}^B = E_2 - E_1.$$

Just for fun, let's compute the normalization factor C^B. The norm of Ψ^B_2 is

$$\int dx_1\cdots dx_N |\Psi^B_2(x_1,\ldots,x_N)|^2 =$$

$$= |C^B|^2 \sum_{i,j=1}^{N} \int dx_1\cdots dx_N \Psi^B_1(x_1,\ldots,x_{i-1},x_{i+1},\ldots,x_N)\varphi_2(x_i)\Psi^B_1(x_1,\ldots,x_{j-1},x_{j+1},\ldots,x_N)\varphi_2(x_j)$$

$$= |C^B|^2 \sum_{i,j=1}^{N} \delta_{ij} = |C^B|^2 \sum_{i=1}^{N} = N|C^B|^2,$$

and therefore $C^B = \frac{1}{\sqrt{N}}$.

(e) **(5 points)** For the case of N identical fermions in the same box, we need to find the lowest-energy eigenstate which is *antisymmetric* under the exchange of any pair of particles. If any two particles are in the same state, then the antisymmetric combination identically vanishes, so each particle must be in a different single-particle energy eigenstate. The lowest possible energy for our N fermion system is thus

$$\mathcal{E}^F_{min} = E_1 + \dots E_N$$

Note that the fermionic ground state has a (much!) higher energy than the bosonic ground state. A simple state with this energy is

$$\Psi_{1,2,\dots N}(x_1, \dots x_N) = \varphi_1(x_1) \dots \varphi_N(x_N)\,, \qquad \mathcal{E}_{\{n_i\}} = \sum_{i=1}^{N} E_i$$

However, this state is not antisymmetric under the interchange of any pair of particles. A completely antisymmetric wavefunction of this form can be constructed by superposing all possible permutations $\{p_i\}$ in which the i^{th} particle is in the ${p_i}^{th}$ state, weighted by a relative sign determined by how many exchanges were involved in that permutation. Explicitly,

$$\Psi^F_1(x_1, \dots x_N) = C^F \sum_p (-1)^{|p|}\, \varphi_{p_1}(x_1)\varphi_{p_2}(x_2) \cdots \varphi_{p_N}(x_N),$$

where p is any permutation of the particles and $|p|$ is the number of exchanges required to turn the permutation into the standard ordering $(1,\dots N)$. By construction, this wave function is totally antisymmetric (check!).

To fix the normalization, C^F, we must compute the norm of Ψ^F_1,

$$\int dx_1 \cdots dx_N |\Psi^F_1(x_1, \dots, x_N)|^2 =$$

$$= |C^F|^2 \sum_p \sum_{p'} (-1)^{|p|}(-1)^{|p'|} \int dx_1 \cdots dx_N\, \varphi^*_{p_1}(x_1) \cdots \varphi^*_{p_N}(x_N)\, \varphi_{p'_1}(x_1) \cdots \varphi_{p'_N}(x_1)$$

$$= |C^F|^2 \sum_p \sum_{p'} (-1)^{|p|}(-1)^{|p'|}\, \delta_{p,p'} = |C^F|^2 \sum_p (-1)^{2|p|} = |C^F|^2 \sum_p = |C^F|^2 N!,$$

where $\delta_{p,p'}$ is equal to 1 when p and p' are the same permutation, and 0 otherwise, and we used the fact that there are $N!$ permutations acting on the N positions. Therefore

$$C^F = \frac{1}{\sqrt{N!}}.$$

To excite this fermionic ground state, we must take of of the identical particles and lift it to the next available single-particle energy eigenstate. The first such available state compatible with antisymmetry of the N-fermion wavefunction is thus φ_{N+1}, so the lowest possible excited energy eigenstate for the N-fermion system must be,

$$\mathcal{E}^F_{first} = E_1 + \dots + E_{N-1} + E_{N+1} \qquad \Rightarrow \qquad \Delta\mathcal{E}^F = E_{N+1} - E_N.$$

Problem 5. (15 Points) Meaning of the Crystal Momentum

(a) **(7 points)** In this problem we consider an electron in a periodic potential with energy spectrum $E(q)$ in a wavepacket with crystal momentum $\hbar q$ propagating with group velocity $v_g = \frac{1}{\hbar}\frac{\partial E(q)}{\partial q}$. If an external force F acts on the electron for a short time Δt, it will do work on the electron and increase its energy:

$$\Delta E = E(q + \Delta q) - E(q) = \frac{\partial E(q)}{\partial q}\Delta q = \frac{1}{\hbar}\frac{\partial E(q)}{\partial q}\Delta(\hbar q). \tag{24}$$

This increase in energy is equal to the work done:

$$W = F\Delta x = F\frac{\Delta x}{\Delta t}\Delta t = F v_g \Delta t. \tag{25}$$

Equating the two expressions, inserting the definition of v_g, and taking the limit $\Delta t \to 0$ gives the desired result:

$$F = \frac{d(\hbar q)}{dt}. \tag{26}$$

(b) **(8 points)** An electron in an allowed energy band is not in a momentum eigenstate, and so does not have a definite momentum or velocity. However, we just proved that this system responds to an imposed force as if there *were* a particle with momentum $\hbar k$ and velocity v_g. We call this object the "quasiparticle". So what is its mass, m_*?

By definition, mass is the ratio of Force to acceleration[2], $F = m_* a$. Since the velocity of our wavepacket is the group velocity $v_g = \frac{1}{\hbar}\frac{\partial E(q)}{\partial q}$, we have

$$a = \frac{dv_g}{dt} = \frac{d}{dt}\left[\frac{1}{\hbar}\frac{\partial E(q)}{\partial q}\right] = \frac{1}{\hbar}\frac{\partial^2 E(q)}{\partial q^2}\frac{dq}{dt} = \frac{1}{\hbar^2}\frac{\partial^2 E(q)}{\partial q^2}F \tag{27}$$

where the last equality used the result from part (a), and in the step before we used the chain rule. Comparing to $F = m_* a$, we find,

$$\frac{1}{m_*} = \frac{1}{\hbar^2}\frac{d^2 E(q)}{dq^2}. \tag{28}$$

[2]Here we are implicitly using Ehrenfest's Theorem: the expectation values of a quantum systems respect the appropriate classical equations of motion. In the above calculations, all quantities can be taken to represent expectation values. NB, you might be tempted to say, "mass is the ratio of momentum to velocity", but that is *not* true when the mass is changing, as is familiar from the classical rocket problem.

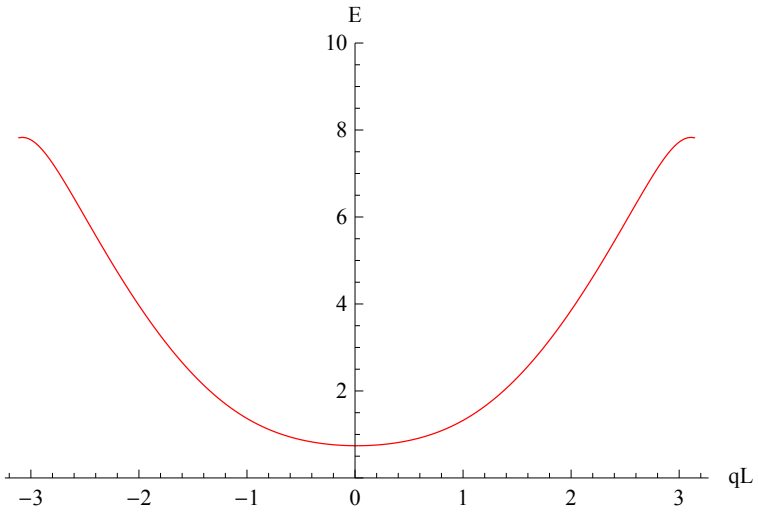
Since $m_* \neq m_e$, the quasiparticles are not simply free electrons. But of course they're not free electrons, the electrons are scattering off a periodic potential! Think back to the ping pong ball experiment described in lecture. The mass of the ping pong ball was much greater than expected due to the interaction between the ping pong ball and the fluid, with the interaction impeding the acceleration of the ping pong ball. Here, similarly, the interaction of the electron with the lattice – in particular, the effect of constructive and destructive interference of the electron wavefunction off all the barriers in the lattice – effectively impedes the acceleration of the electron.

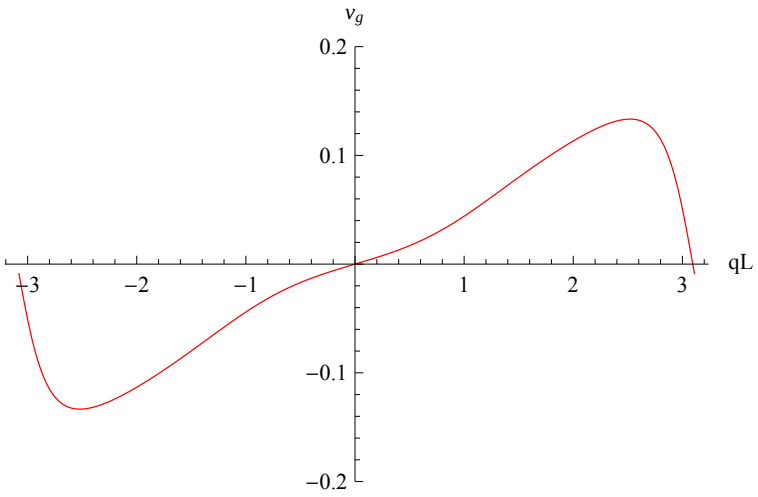
Problem 6. (15 Points) The Group Velocity and Effective Mass

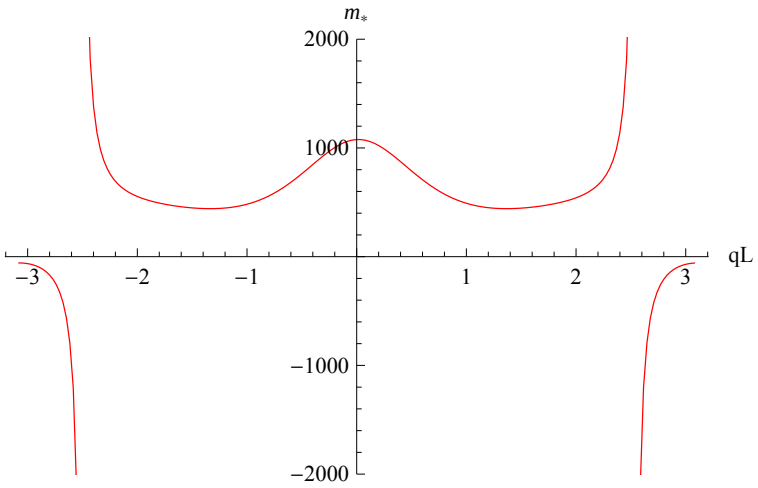
(a) **(7 points)** To sketch v_g and m_*, we simply use the expressions from the previous problem,

$$v_g = \frac{1}{\hbar}\frac{\partial E(q)}{\partial q} \quad \text{and} \quad m_* = \hbar^2 \left[\frac{d^2E(q)}{dq^2}\right]^{-1}, \tag{29}$$

taking the necessary derivatives of $E(q)$. Shown below are the plots for $E(qL)$, $v_g(qL)$ and $m_*(qL)$, with the vertical axes once again plotted in arbitrary units:







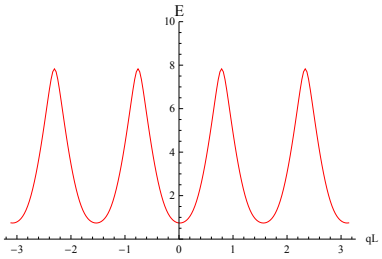
From these graphs, one can see that

- At the bottom of each band, $v_g = 0$ and the wavefunctions are standing wave solutions. The effective mass m_* is positive.
- In the middle of a band, v_g is non-zero and can be either positive or negative. This corresponds to traveling wave solutions. The effective mass m_*, likewise, may be positive or negative, and at one point diverges!
- At the top of each band, $v_g = 0$ and we once again have standing wave solutions. The effective mass m_* is negative.

(b) **(8 points)** The force experienced by an electron in a uniform electric field $\mathcal{E}$ is given by $-e\mathcal{E}$. Integrating the expression $F = d(\hbar q)/dt$ gives

$$\hbar q = -e\mathcal{E}t, \tag{30}$$

where we have omitted the integration constant because we are told that the electron sits initially at the *bottom* of an unoccupied band (so $q = 0$ initially). As the electron is accelerated, then, the quantity qL increases linearly, and we can read off $E(qL)$ and $v_g(qL)$ from our graphs. Now, recall that all the graphs in the previous part were periodic in qL with period 2π. The graph for $E(qL)$, for example, looks like this:



Thus, both the electron's energy and its velocity v_g oscillate.

The velocity of the electron changes in a way that may naively seem to violate the conservation of momentum. However, the electron is not a free particle, and interacts with the lattice. Momentum is therefore exchanged between the electron and the lattice, and thus *total* momentum is conserved.

More precisely, consider what happens to the momentum $m_* v_g$ as our quasiparticle is accelerated. Near the bottom of the band, the mass is positive and the velocity increases with time, so the momentum increases too – the quasiparticle behaves just like an electron, albeit with a slightly modified mass. As we approach the middle of the band, the effective mass grows large, which means the acceleration induced by the constant EMF becomes small – and indeed the velocity approaches its maximum. As we pass the middle of the band, a remarkable thing happens – the mass becomes (infinitely) negative, which means our quasiparticle should accelerate in the *opposite* direction as the external force – and indeed, above the midpoint, the velocity begins to get *smaller*! Continuing to the top of the band, the mass becomes a small negative number and the velocity approaches zero, accelerating precisely as we'd expect given the EMF and the magnitude of the mass but in the opposite direction – it behaves like a positively charged quasiparticle with positive mass $|m_*|$. As we continue following the quasiparticle, it reverses its trajectory, accelerating down the band and returning to the bottom to repeat the cycle.

Now consider what happened to the momentum $m_* v_g$ during this cycle. At any moment of time, though m_* and v_g might change sign, the change in the total momentum, $\delta(m_* v_g)$ is always strictly positive, and indeed equal to the incident force. So while velocity is certainly not conserved, nor energy, the *crystal momentum* is.

Note that all of the preceding discussion hinged on the fact that our quasiparticle (*née* electron) was in an unfilled band, and could therefore move "freely" between energy states within a band and change velocity in response to an external electric field. In a metal, in which the valence band is partially filled, we must deal with the complexities of many-electron systems. With insulators, on the other hand, the outermost electrons are typically at the top of a filled band, so the electron cannot change its energy at all unless the external force imparts enough energy to kick it across the gap.

Problem Set 10 **Solutions**
8.04 Spring 2013 **Thursday, May 9**

Problem 7. (35 Points) Transmission, Reflection and Bandgaps in 1d

(a) **(4 Points)** The scattering phases are defined[3] so that

$$t = \sqrt{T}e^{-i\varphi} \quad \text{and} \quad r = \pm i\sqrt{R}e^{-i\varphi} \tag{31}$$

We are also given that

$$\cos qL = \frac{t^2 - r^2}{2t}e^{ikL} + \frac{1}{2t}e^{-ikL}. \tag{32}$$

First we find $t^2 - r^2$:

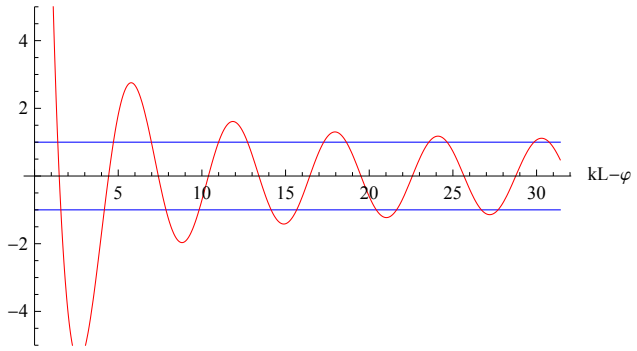
$$t^2 - r^2 = Te^{-i2\varphi} + Re^{-i2\varphi} = e^{-i2\varphi}, \tag{33}$$

where we have used the fact that $T + R = 1$, by definition. Substituting this into Equation 32 gives

$$\cos qL = \frac{1}{2t}\left(e^{-i2\varphi}e^{ikL} + e^{-ikL}\right) = \frac{1}{2\sqrt{T}}\left(e^{ikL-i\varphi} + e^{-ikL+i\varphi}\right) = \frac{\cos(kL-\varphi)}{\sqrt{T}}, \tag{34}$$

which is our desired result.

(b) **(4 Points)** Since $T < 1$, the RHS of Equation 34 has always modulus greater than 1 in some neighborhood of $kL - \varphi = n\pi$. Below is shown a plot of the RHS of 34 plotted against $kL - \varphi$:

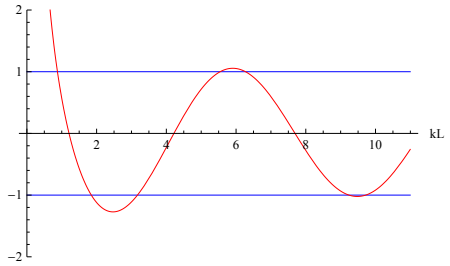


Since the L.H.S. of Equation 34 must be between -1 and $+1$, only regions where the red curve is between the two blue horizontal lines will solutions exist. We can see

[3]See eg Liboff's discussion of 1d scattering. For a nice discussion of scattering in 1d which goes a bit beyond what we've done, see eg these lecture notes by Ben Simons or the very thorough but readable discussion in Elementary Quantum Mechanics in One Dimension by R. Gilmore (not D. Waters of P. Floyd, though that's an excellent resource for diffraction, too). For a more formal and terse discussion, see J. H. Eberly, Quantum Scattering Theory in One Dimension, American Journal of Physics 33 (1965) 10 pp.771.

from the plot that the gap regions (where no solutions exist) occur at the "peaks" and "valleys" of the curve, which because of the cosine dependence of the R.H.S. of Equation 34 occur at roughly $kL - \varphi = n\pi$.
From the above result, we can say that φ sets the global position of the gaps of the band structure. In other words, shifting φ corresponds to an overall shifting of the gaps positions.

(c) **(6 Points)** If the barriers are very weak, we expect excellent transmission ($T \approx 1$) and poor reflection ($R \approx 0$). We also expect the phase shift to be small (consider a situation where we slowly dial the strength of the potential down to zero — we expect the phase shift to continuously go to zero). In this limit, our plot looks like this:



The gap regions (the parts that poke below -1 and above $+1$) are narrow and are found in regions close to $kL \approx n\pi$. Since the gaps are narrow we can solve for the intersections by Taylor expanding Equation 34 about $kL = n\pi$:

$$\frac{\cos kL}{\sqrt{T}} = \frac{\cos(n\pi \pm \varepsilon)}{\sqrt{T}} \approx \frac{\cos(n\pi) \mp \varepsilon \sin n\pi - \frac{\varepsilon^2}{2}\cos n\pi \mp \dots}{\sqrt{T}} = \frac{(-1)^n(1 - \frac{\varepsilon^2}{2} + \dots)}{\sqrt{T}}. \tag{35}$$

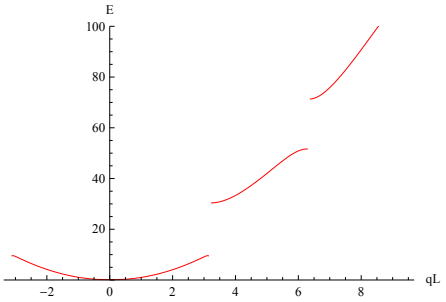
From the graph, we can see that for odd n the lines intersect at $\cos qL = -1$ wheres for even n they intersect at $\cos qL = +1$. The $(-1)^n$ factor therefore cancels the ± 1 on the L.H.S. of Equation 34, and we have

$$1 \approx \frac{1 - \frac{\varepsilon^2}{2}}{\sqrt{T}} \qquad \Rightarrow \qquad \sqrt{T} \approx 1 - \frac{\varepsilon^2}{2} \tag{36}$$

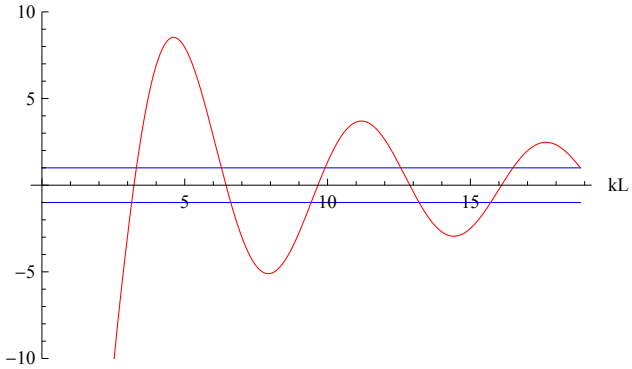
Using $\sqrt{T} = \sqrt{1 - R} \sim 1 - R/2$, then plugging into the above, thus gives,

$$\varepsilon \approx \sqrt{R}\,. \tag{37}$$

where we have used the fact that $T + R = 1$ and that R is small in the limit of weak barriers. We see that for weak barriers the width in kL of the gaps are proportional to $\sqrt{R}$. In the plot below we show $E(q)$ (with the vertical axis in arbitrary units) as a function of qL for a system like this:



(d) **(7 Points)** In the limit of strong barriers, we expect low transmission (T small), high reflection ($R \approx 1$) and the phase shift to be approximately $\pi/2$. From the plot on the next page, we can see that the energy bands are narrow, and centered around $kL = n\pi$.



Once again, this suggests that we can use a Taylor series expansion to approximate the behavior around $kL = n\pi$:

$$\frac{\cos(kL+\delta)}{\sqrt{T}} = \frac{\cos(kL+\frac{\pi}{2})}{\sqrt{T}} = \frac{\cos kL\cos\frac{\pi}{2} - \sin kL\sin\frac{\pi}{2}}{\sqrt{T}} = -\frac{\sin kL}{\sqrt{T}} \tag{38a}$$

$$= -\frac{\sin(n\pi+\varepsilon)}{\sqrt{T}} \approx -\frac{\sin n\pi - \varepsilon\cos n\pi + \ldots}{\sqrt{T}} \tag{38b}$$

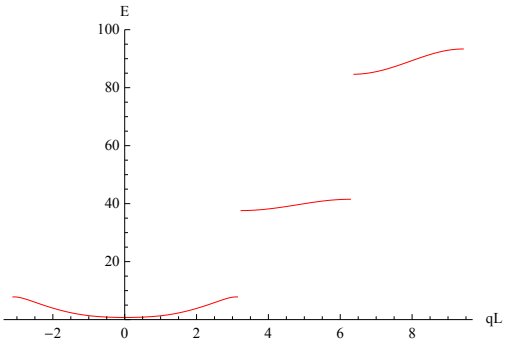
$$\approx (-1)^n\frac{\varepsilon}{\sqrt{T}}. \tag{38c}$$

With $\varepsilon > 0$ (*i.e.* for the top edge of the band) the curve to intersect is $(-1)^n$, so the minus signs once again cancel, giving

$$\frac{\varepsilon}{\sqrt{T}} = 1 \quad \Rightarrow \quad \varepsilon = \sqrt{T}, \tag{39}$$

so the width of kL in the energy band is directly proportional to $\sqrt{T}$.

Above we show a typical plot of $E(q)$ that results from this strong barrier limit, once again with the vertical axis in arbitrary units and the horizontal axis in units of qL.



(e) **(7 Points)** In Problem Set 7, we analyzed scattering off a single delta function, and found that the ratio of the transmitted amplitude to the incident amplitude was

$$\frac{C}{A} = \frac{1}{1 - i\frac{mV_0}{\hbar^2 k}}. \tag{40}$$

To translate to the notation used in this problem, we need to make the replacement $V_0 \to -\frac{\hbar^2 g_o}{2mL}$. Moreover, the ratio C/A is the quantity t defined in this problem by the equation

$$t = \sqrt{T}e^{-i\varphi}. \tag{41}$$

We therefore have

$$t = \frac{1}{1 + i\frac{g_o}{2kL}} = \frac{1 - i\frac{g_o}{2kL}}{1 + \left(\frac{g_o}{2kL}\right)^2}. \tag{42}$$

Comparing the last two equations and using $e^{-i\varphi} = \cos(\varphi) + i\sin(\varphi)$, we see that

$$\cot\varphi = -\frac{2kL}{g_o}. \tag{43}$$

Similarly, the transmission coefficient is given by

$$T = \frac{\left(\frac{2kL}{g_o}\right)^2}{1 + \left(\frac{2kL}{g_o}\right)^2} = \frac{\cot^2\varphi}{1 + \cot^2\varphi} = \frac{\cot^2\varphi}{\csc^2\varphi} = \cos^2\varphi. \tag{44}$$

Let us now insert everything into Equation 34. The L.H.S. is already in the form we want, so we consider the R.H.S.:

$$\frac{\cos(kL - \varphi)}{\sqrt{T}} = \frac{\cos kL\cos\varphi + \sin kL\sin\varphi}{\cos\varphi} =$$

$$= \cos kL + \cot\varphi\sin kL = \cos kL + \frac{g_o}{2kL}\sin kL, \tag{45}$$

and thereby arrive at the familiar result:

$$\cos qL = \cos kL + \frac{g_o}{2kL}\sin kL. \tag{46}$$

(f) **(7 Points)** Since the energy $E = \frac{\hbar^2 k^2}{2m}$ is a real number, we want k to be either real or purely imaginary. For either sign of g_o, the equation we need to solve is always

$$\cos qL = \cos kL + \frac{g_o}{2kL} \sin kL. \tag{47}$$

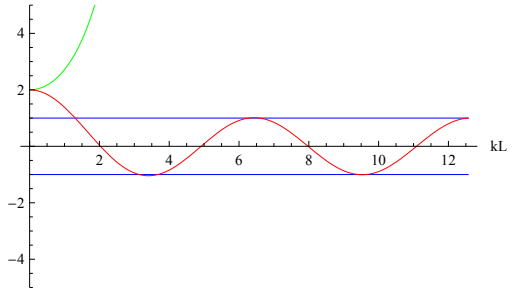
When k is imaginary, it's more convenient to define $\kappa = -ik$, and the above equation translates into

$$\cos qL = \cosh \kappa L + \frac{g_o}{2\kappa L} \sinh \kappa L. \tag{48}$$

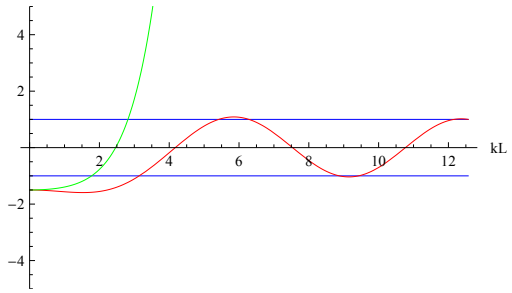
Therefore, regarding both k and κ as real, (47) gives us solutions corresponding to positive energy, and (48) accounts for solutions with negative energy, because

$$E = \frac{\hbar^2 k^2}{2m} = -\frac{\hbar^2 \kappa^2}{2m} < 0.$$

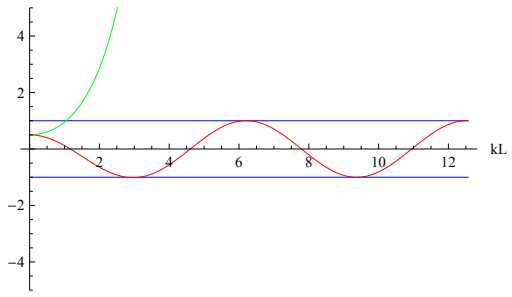
There are three different regimes for this problem: $g_o > 0$, $g_o < -4$ and $-4 < g_o < 0$. In the previous parts we explored the first case, for which we know that there are no bound states, and this fact corresponds to having no solutions to equation (48). This can be seen from the following plot, where $g_o = 2$.



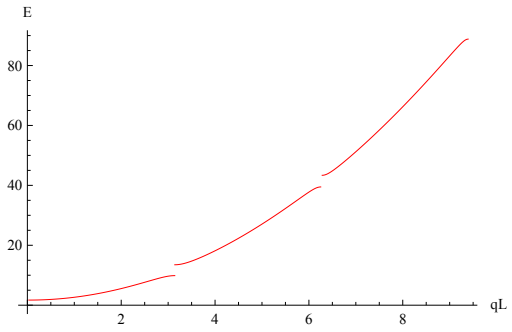
The red curve is the plot of the RHS of (47), and the green curve is the plot of the RHS of (48). Note that the green curve lies outside the horizontal stripe between -1 and 1, and this corresponds to the fact that we don't have solutions to (48). In the second case the plot is as follows, with $g_o = -5$:

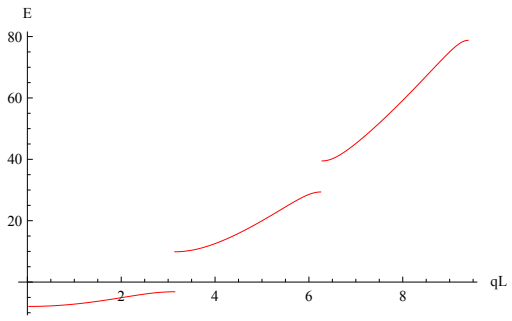


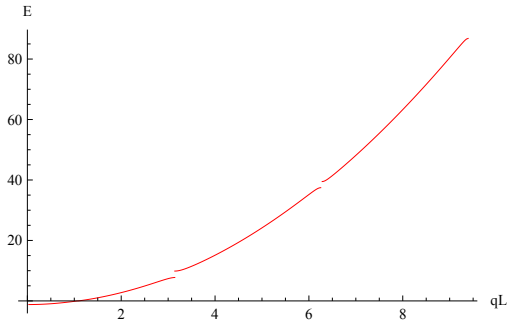
Note that now also the green curve has an overlap with the horizontal stripe, so that we have solutions to (48). These solutions correspond to a band of bound states, which is always just one, no matter how negative g_o, and we have multiple bands for positive energy states, which correspond to the overlaps of the red curve with the horizontal stripe. The case when $-4 < g_o < 0$ is represented in the following plot, with $g_o = -1$:



which corresponds to the fact that there is one band which is composed partially by bound states and partially by positive energy states. Below are the plots of $E(q)$ corresponding to the three different cases.







Problem Set 10 **Solutions**
8.04 Spring 2013 **Thursday, May 9**

Problem 8. (OPTIONAL) Standing Waves at the Band Edges

Before tackling this problem, let us first remind ourselves of the system we studied in lecture. The potential was a periodic series of delta functions:

$$V(x) = \sum_{s=-\infty}^{\infty} \frac{\hbar^2}{2m}\frac{g_o}{L}\delta(x - sL). \tag{49}$$

Between the delta function barriers, the solution to the Schrödinger equation takes the form

$$\psi_E(x) = Ae^{ikx} + Be^{-ikx}, \tag{50}$$

where $E = \frac{\hbar^2 k^2}{2m}$. Since the potential is periodic, we expect the probability distribution for energy eigenstates to also be periodic; however, **the wavefunction is not periodic**, but rather satisfies the condition,

$$\psi_E(x + L) = e^{iqL}\psi_E(x), \tag{51}$$

where q is known as the *crystal momentum*. By imposing continuity on the wavefunction and the jump condition on the slope, plus the non-periodicity condition, we get

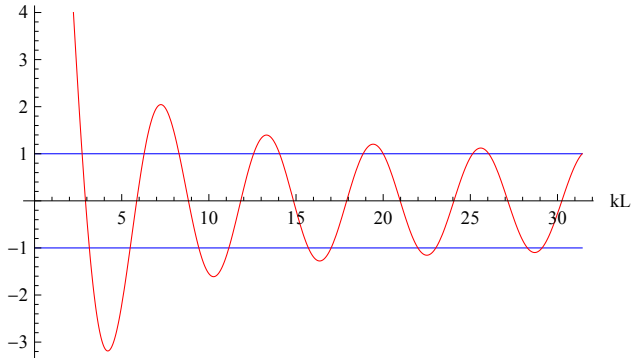
$$A + B = Ae^{i(k-q)L} + Be^{-i(k+q)L} \tag{52a}$$

$$\frac{g_o}{L}(A + B) = ik(A - B) - ik\left[Ae^{i(k-q)L} - Be^{-i(k+q)L}\right]. \tag{52b}$$

Eliminating A and B from Equations 52a and 52b gives

$$\cos qL = \cos kL + \frac{g_o}{2kL}\sin kL. \tag{53}$$

Since $\cos qL$ falls between $+1$ and -1, we can solve this equation as follows:
The above is a plot of the R.H.S. of Equation 53 [red line] and of the lines $y = \pm 1$ [blue lines] with the dimensionless parameter g_o set to 13. A solution will only exist if the red line falls between the two blue lines. The regions along the k-axis where this is the case correspond to allowed energy *bands*, and are separated by disallowed *gap* regions. The edges of the bands are given by the intersections of the red curve and the blue curves, and correspond to setting $qL = N\pi$ so that $\cos qL = \pm 1$. For instance, in this example the first energy band runs from $kL \approx 2.73$ to $kL = \pi$, with the actual energies given by $E = \frac{\hbar^2 k^2}{2m}$.

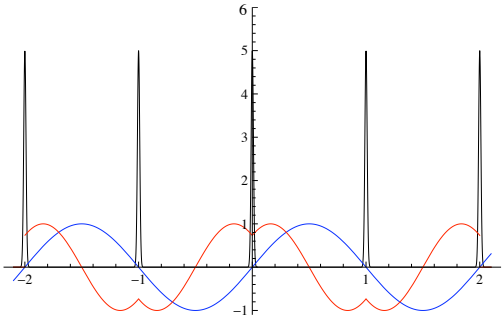


(a) As we mentioned above, regardless of the value of g_o, the top edge of an energy band (or equivalently the bottom energy of an energy gap) will be at $qL = N\pi$, where N is some integer not equal to zero.

(b) In the absence of a potential, ie for free particles, the two energy eigenfunctions with $qL = N\pi$ would simply be $\sin(N\pi x/L)$ and $\cos(N\pi x/L)$. Turning on the periodic delta function potential with $g_o > 0$ gives these eigenfunctions a kink satisfying:

$$\phi'_E(nL^+) - \phi'_E(nL^-) = \frac{g_o}{L}\phi_E(nL), \tag{54}$$

Since $\sin(N\pi x/L)$ vanishes at each delta function, the right hand side becomes zero and the slope becomes continuous, so the delta functions have no effect. Since $\cos(N\pi x/L)$ does not vanish at the delta functions, they induce kinks at the barriers. For $N = 1$:



The blue eigenstate has zeros at the delta function sites and therefore does not "see" the barriers. It is therefore a free particle state. The red eigenstate, however, *does* see the delta functions and has kinks in its wavefunction. It corresponds to a higher energy state because it has a greater curvature than the blue curve. Note that these two eigenfunctions *do not* belong to the same band: the blue curve corresponds to the top state of some energy band, while the red curve corresponds to the bottom edge of the *next* energy band (equivalently, the blue curve is the bottom of the first gap, while the red curve is the top of the first gap). However, as the strength of the barriers goes to zero, the kinks go away and these two state – the top of the first band and the bottom of the second – become sine and cosine wavefunctions with the same curvature, and thus the same energy – ie, the gap closes and the bands merge.

When $g_o \to \infty$, the value of $\phi_E(nL)$ goes to zero in such a way that the RHS of 54 tends to a finite constant, and thus the jump of the derivative of the even function represented in red in the previous plot remains finite. Therefore, in the $g_o \to \infty$ limit, all the states vanish at $x = nL$, and between two delta functions they look like a free particle with momentum $N\pi/L$. Note that, among these states, there is only one that is a true momentum eigenstate, which is $\sin\left(x\frac{N\pi}{L}\right)$.

(c) At $x = 0$, the wavefunction must be continuous:

$$\phi_E(0^-) = \phi_E(0^+), \tag{55}$$

while its slope jumps because of the presence of the delta function:

$$\phi'_E(0^+) - \phi'_E(0^-) = \frac{g_o}{L}\phi_E(0). \tag{56}$$

Since we are dealing with a periodic potential, we know from the preamble that

$$\phi_E(x + L) = e^{iqL}\phi_E(x). \tag{57}$$

In this problem we are interested in the band edges $qL = N\pi$, so $e^{iqL} = (-1)^N$, so

$$\phi_E(x + L) = (-1)^N\phi_E(x). \tag{58}$$

(d) Since the potential is zero away from the locations of the delta functions, we can say $\phi_E(x) = A\sin(kx + \theta)$ in the region $0 < x < L$, where $E = \frac{\hbar^2k^2}{2m}$. Our boundary conditions, however, require the evaluation of the wavefunction and its derivative at places like $x = 0^-$, which lies outside the region. We must therefore use Equation 58 to obtain the form of the eigenfunction for $-L < x < 0$. This yields

$$\phi_E(x) = \begin{cases} (-1)^N A\sin\left[k(x + L) + \theta\right] & \text{for } -L < x < 0 \\ A\sin(kx + \theta) & \text{for } 0 < x < L. \end{cases} \tag{59}$$

We can now begin to impose our boundary conditions. The condition $\phi_E(0^+) = \phi_E(0^-)$ becomes

$$A\sin\theta = (-1)^N A\sin(kL + \theta) \quad \Rightarrow \quad \boxed{\sin\theta = (-1)^N\sin(kL + \theta)}\,. \tag{60}$$

The jump condition requires us to find the derivatives

$$\phi'_E(0^+) = Ak\cos\theta \tag{61a}$$
$$\phi'_E(0^-) = (-1)^N Ak\cos(kL + \theta). \tag{61b}$$

which give

$$\boxed{\cos\theta - (-1)^N\cos(kL + \theta) = \frac{g_o}{kL}\sin(\theta)}\,. \tag{62}$$

(e) Our goal is now to find solutions to the boxed equations above,

$$\sin\theta = (-1)^N \sin(kL+\theta) \tag{63a}$$

$$\cos\theta - (-1)^N \cos(kL+\theta) = \frac{g_o}{kL}\sin(\theta). \tag{63b}$$

Using $\sin(-x) = -\sin(x)$, Equation 63a can be written as

$$\sin\theta = \sin[(-1)^N(kL+\theta)]. \tag{64}$$

If we "simplify" the sin in Equation 64, we obtain

$$\theta = (-1)^N(kL+\theta) + 2M\pi, \tag{65}$$

or

$$\pi - \theta = (-1)^N(kL+\theta) + 2M\pi, \tag{66}$$

where the second Equation comes about by taking into account that $\sin x = \sin(\pi - x)$. By plugging in and evaluating, it is immediately clear that $\theta = 0$ and $qL = N\pi$ furnish one set of solutions. However, it is illuminating (and will be useful shortly) to derive this solution rather than check it. The following table shows the solutions we get from the first and the second Equations above.

	N even	N odd
Eq. 65	$kL = -2M\pi$	$kL = -2\theta + 2M\pi$
Eq. 66	$kL = -2\theta - (2M-1)\pi$	$kL = (2M-1)\pi$

As we can see, half of the solutions come form $kL = M\pi$. Now we need to check that only $\theta = 0$ is compatible with these solutions, and we shall do it by considering Equation 63b. Inserting in the latter $kL = -2M\pi$ for N even, we obtain

$$\cos\theta - \cos(-2M\pi + \theta) = \frac{g_o}{kL}\sin(\theta), \tag{67}$$

and, since the LHS is zero, we obtain $\theta = 0$, as expected. For N odd, plugging $kL = (2M-1)\pi$ in Equation 63b we obtain

$$\cos\theta + \cos((2M-1)\pi + \theta) = \frac{g_o}{kL}\sin(\theta), \tag{68}$$

recalling that $\cos(x-\pi) = -\cos(x)$, we again obtain that the LHS is zero, and thus $\theta = 0$.

States with $kL = N\pi$ and $\theta = 0$ are of the form $\phi_E = (x) = A\sin kx$. These energy eigenfunctions have the infinite-well energy $E = N^2\frac{\hbar^2\pi^2}{2mL^2}$ and *vanish* at the delta functions. These are precisely the states we argued in part (a) would appear at the *top* of each energy band, ie at the *bottom* of each gap.

(f) From the table in part (d), we know what the other half of the solutions are

$$kL = -2\theta - (2M-1)\pi \qquad \text{for } N \text{ even}, \tag{69}$$

$$kL = -2\theta + 2M\pi \qquad \text{for } N \text{ odd}, \tag{70}$$

Proceeding as before, let's take N even and recast into Equation 63b,

$$\cos\theta - \cos(-\theta - 2M\pi + \pi) = \frac{g_o}{kL}\sin\theta, \tag{71}$$

from which we can write

$$2\cos\theta = \frac{g_o}{kL}\sin\theta, \tag{72}$$

thus

$$\cot\theta = \frac{g_o}{2kL}, \tag{73}$$

and, using 69,

$$\cot\left(\frac{kL}{2}\right) = \cot\left(-\theta - M\pi + \frac{\pi}{2}\right) = \tan\theta = \frac{1}{\cot\theta} \tag{74}$$

where we used

$$\cot(x-\pi) = \cot(x), \qquad \cot\left(\frac{\pi}{2} - x\right) = \tan(x). \tag{75}$$

Thus, finally

$$\cot\left(\frac{kL}{2}\right) = \frac{g_o}{2kL}. \tag{76}$$

For N odd, we insert 70 in Equation 63b and get

$$\cos\theta + \cos(-\theta + 2M\pi) = \frac{g_o}{kL}\sin\theta, \tag{77}$$

and thus

$$\cot\theta = \frac{g_o}{2kL}. \tag{78}$$

Now, from Equation 70,

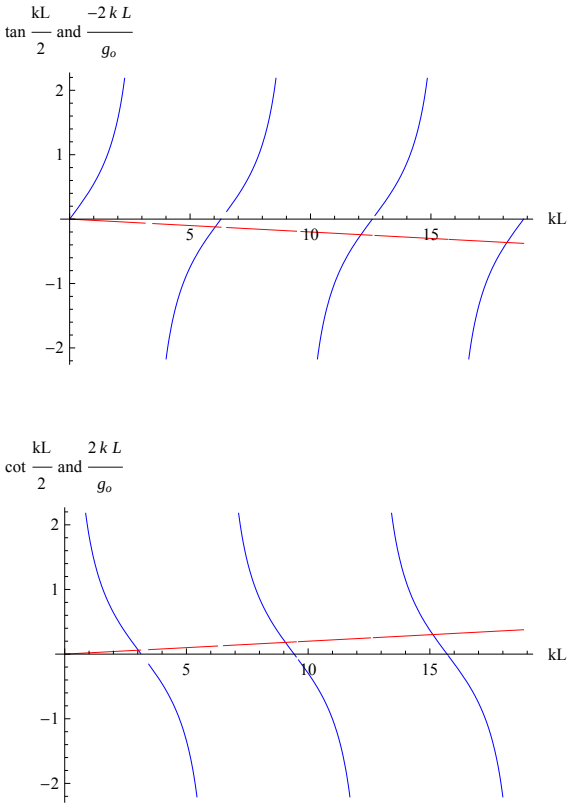
$$\tan\left(\frac{kL}{2}\right) = \tan(-\theta + M\pi) = -\tan\theta = -\frac{1}{\cot\theta}, \tag{79}$$

where we used the first identity in 75, and thus

$$\tan\left(\frac{kL}{2}\right) = -\frac{2kL}{g_o}. \tag{80}$$

These states appear at the *bottom* of the band.

(g) Shown below are plots of Equations 76 and 80 for large values of g_o. The left hand side of each equation is plotted in blue, while the right hand side is red:

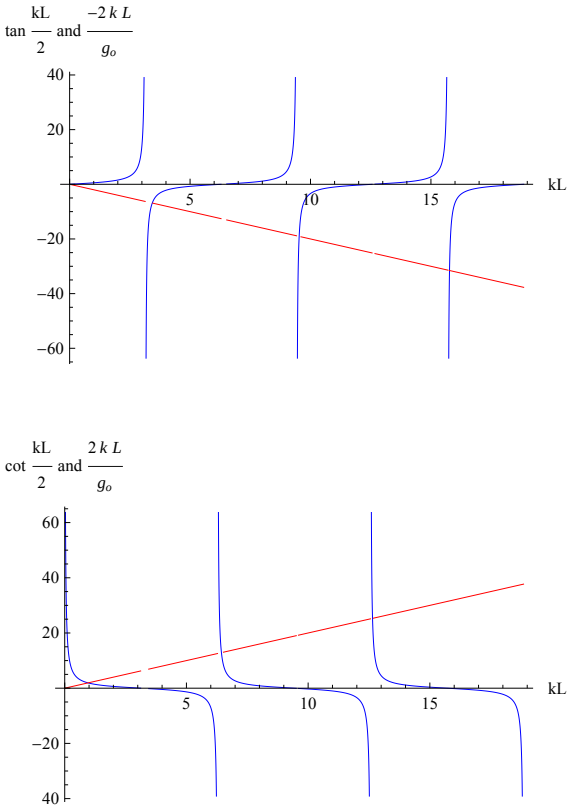


One can see that as $g_o \to \infty$, the solutions coming from these graphs (given by the intersections between the red and blue lines) approach multiples of π from below (*i.e.* as g_o goes up, the solution kL's increase and approach multiples of π). Now, recall from before that these solutions correspond to the *bottom* edges of energy bands, and that the *top* edges are fixed at multiples of π irrespective of the value of g_o. We can therefore conclude that as g_o is increased, the sizes of the bands go to zero. As $g_o \to \infty$, the gaps get correspondingly larger, and asymptote to

$$\Delta E_{gap} = \frac{\pi^2 \hbar^2}{2mL^2} \left[(n+1)^2 - n^2 \right], \tag{81}$$

This makes sense because the eigenstates approach the free particle states and the energy levels become degenerate in infinitely thin "bands" corresponding to the energy levels of an infinite well as $g_o \to \infty$.

(h) Here we show the analogous plots for small values of g_o:



These solutions (which, remember, are the *bottom* edges of the bands) are seen to approach multiples of π *from above* as we dial $g_o \to 0$. In other words, as $g_o \to 0$, these band edges move *away* from the top edges of their own bands (which are given by the *next* multiple of π), and approach the top edges of the bands below them. As $g_o \to 0$, the gaps therefore close completely, and all energies are allowed. This makes sense, because with $g_o = 0$, the barriers are non-existent and we only have free particle solutions, which form a continuum of energy states.

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8.04 Quantum Physics I

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