Professor Allan Adams

Problem Set 10

Due Friday May 10 at 11.00AM

Assigned Reading:

E&R	$13_{1..7}$
Li.	$8_{1..4}$
Ga.	$4_{supplements}$, 13_{all}
Sh.	*see Liboff*

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

   Consider a particle of mass m in a lattice of delta function barriers of dimensionless strength $g_o \gg 1$, lattice spacing L, and total length $D \gg L$. Estimate the ground state energy and compare it to that of a particle confined to a box of width D.

2. **(5 points) Blinded by Science**

   Diamond, with a band gap of $5.5eV$, is a spectacular insulator: at room temperature, diamond sports roughly 10^{-44} times fewer electrons in its conduction band than silicon (bandgap $1.1eV$). Diamond is also famously, and expensively, translucent. What is the minimum frequency to which diamond is opaque? What kind of radiation is this (*e.g.* X-rays, radio, etc)? Curiously, some diamonds are tinted blue. Can you come up with a mechanism that would explain this observation?

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

   Consider a composite object such as the hydrogen atom. Will it behave as a boson or fermion? Argue in general that objects containing an even/odd number of fermions will behave as bosons/fermions.

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

Consider two variables, x_1 and x_2. A natural question is whether knowledge of one variable is predictive of the second variable. Such a predicitivity is called a correlation. *In terms of expectation values, a natural measure of the correlation of the two variables is the* correlator,

$$\langle\, (x_1 - \langle x_1\rangle)\ (x_2 - \langle x_2\rangle)\, \rangle$$

This problem will explore the interplay between symmetry and correlation of variables.

Suppose we carefully arrange two particles in a harmonic oscillator potential such that one is in the ground state ϕ_0 and one is in the first excited state ϕ_1. The following are three wavefunctions in which our two particles may find themselves, corresponding to distinguishable, bosonic (symmetric) and fermionic (anti-symmetric) particles:

$$\begin{aligned}
\psi_D(x_1, x_2) &= \phi_0(x_1)\phi_1(x_2) \\
\psi_S(x_1, x_2) &= \frac{1}{\sqrt{2}} \left(\phi_0(x_1)\phi_1(x_2) + \phi_0(x_2)\phi_1(x_1)\right) \\
\psi_A(x_1, x_2) &= \frac{1}{\sqrt{2}} \left(\phi_0(x_1)\phi_1(x_2) - \phi_0(x_2)\phi_1(x_1)\right) ,
\end{aligned}$$

where

$$\phi_0(x) = \sqrt{\frac{1}{\rho\sqrt{\pi}}} e^{-x^2/2\rho^2} \qquad \phi_1(x) = \sqrt{\frac{2}{\rho\sqrt{\pi}}} \left(\frac{x}{\rho}\right) e^{-x^2/2\rho^2} .$$

(a) Verify that $\langle x_1 \rangle = 0$ and $\langle x_2 \rangle = 0$ in all three cases.

(b) Compute the mean square distance in each of these states and verify that:

$$\begin{aligned}
\psi_S : &\qquad \langle\, (x_1 - x_2)^2 \rangle = 1\rho^2 \\
\psi_D : &\qquad \langle\, (x_1 - x_2)^2 \rangle = 2\rho^2 \\
\psi_A : &\qquad \langle\, (x_1 - x_2)^2 \rangle = 3\rho^2
\end{aligned}$$

Give a physical interpretation to your results. Do the particles in these various states experience different forces? If so, explain why; if not, what is causing the particles to attract or repel?

(c) Plot the probability density associated to each of the three wavefunctions as a function of x_1 and x_2. Do your plots reproduce your conclusion above? What do you see on the slice $x_1 = x_2$?

(d) Suppose your lab partner places N identical bosons of mass μ in an infinite square well of width L, cooling them into the lowest allowed energy eigenstate. What is the wavefunction, $\Psi(x_1, \ldots, x_N)$, of this lowest-energy state in terms of the single-particle states, $\varphi_n(x)$, what is its energy, and what is the minimum energy you must add to the system to excite it into the next allowed energy eigenstate?

(e) Repeat (d) for N identical fermions. Be careful to normalize your wavefunction.

5. **(15 points) Meaning of the Crystal Momentum**

   Consider an electron in a periodic potential with energy spectrum $E(q)$ in a wavepacket with crystal momentum $\hbar q$ propagating with the group velocity $v_g = \frac{1}{\hbar}\frac{\partial E(q)}{\partial q}$.

   (a) Suppose a force F acts upon our system. Use elementary physics (like conservation of energy and the fact that E is a function of q) to show that

   $$\frac{d\,\hbar q}{dt} = F \; .$$

   This is the significance of the crystal momentum, $\hbar q$: it is not the momentum *of the electron, since the electron is not in a momentum eigenstate; however, the crystal momentum, $\hbar q$,* is *the momentum which appears in the law of momentum conservation.*

   (b) Let's dig deeper – if $\hbar q$ is not the momentum of our electron, whose momentum is it? Suppose that this momentum is really the momentum of some particle-like object in our system (let's call it "the quasiparticle") with some effective quasiparticle mass m_* and group velocity v_g. Use Newton's law to show that

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

   Are the quasiparticles plain old electrons? If not, what are they?

6. **(15 points) The Group Velocity and Effective Mass**

   Consider again our lattice of delta functions.

   (a) Sketch $v_g(qL)$ and $m_*(qL)$ for $|qL| < \pi$ in the first two bands. What happens to v_g and m_* near the top of each band? What about in the middle of the band?

   (b) Consider an electron at the bottom of an otherwise unoccupied band. Now accelerate it with a uniform external electric field, $\mathcal{E}$. Show that the crystal momentum increases linearly in time. Qualitatively, what will happen to the energy $E(q)$ and velocity $v_g(q)$ of the wavepacket as a function of time? How does your result fit with conservation of momentum, or the fact that metals (solids with unfilled bands) *conduct* in response to an EMF $\mathcal{E}$?

7. **(35 points) Transmission, Reflection and Bandgaps in 1d**

Band structure is intimately connected to scattering. As discussed in lecture, the existence of gaps is a consequence of destructive interference between waves reflected from distant wells in the lattice. In this problem we'll further develop the connection between scattering and band structure in 1d by using the transmission and reflection coefficients of a single isolated potential to derive the band structure of a lattice of identical such potentials. Let's start by looking at a single barrier in detail.

Single Barrier Scattering

Consider an arbitrary (but reasonable) potential barrier described by a symmetric function $V(x)$ which is zero outside a region of width L centered on the origin, and varies in some simple but non-trivial way between $x = -L/2$ and $x = +L/2$. Now send a beam of particles of mass m and energy $E = \frac{\hbar^2 k^2}{2m}$ towards this barrier from the left. Outside the barrier, where the potential vanishes and the energy eigenvalue equation reduces to that of a free particle, ϕ takes the form,

$$\phi_{\rightarrow}(x) = \left\{ \begin{array}{cc} e^{ikx} + r\,e^{-ikx} & x \leq -\frac{L}{2} \\ t\,e^{ikx} & x \geq +\frac{L}{2}\,. \end{array} \right\}$$

Here, $t = \sqrt{T}e^{-i\varphi}$ and $r = \pm i\sqrt{R}e^{-i\varphi}$ are the familiar transmission and reflection amplitudes, T and R are the trans/reflection probabilities and φ is the phase shift. Similarly, sending particles in from the right at the same energy E gives,

$$\phi_{\leftarrow}(x) = \left\{ \begin{array}{cc} t\,e^{-ikx} & x \leq -\frac{L}{2} \\ e^{-ikx} + r\,e^{ikx} & x \geq +\frac{L}{2} \end{array} \right\}$$

with the same t and r due to the symmetry of the potential, $V(x) = V(-x)$.

A general energy eigenfunction ϕ_E with energy E can then be expressed as a superposition of these two scattering solutions,

$$\phi_E(x) = \mathcal{A}\,\phi_{\rightarrow}(x) + \mathcal{B}\,\phi_{\leftarrow}(x)$$

A Lattice of Identical Scatterers

Now consider a lattice of such barriers. Bloch's Theorem says that we can find energy eigenstates which satisfy the periodicity condition,

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

Taking a derivative with respect to x, this also implies

$$\phi'_E(x+L) = e^{iqL}\phi'_E(x)\ .$$

Meanwhile, from our study of the single well solutions above, we also know that $\phi_E(x) = \mathcal{A}\,\phi_{\rightarrow}(x) + \mathcal{B}\,\phi_{\leftarrow}(x)$, where $\phi_{\rightarrow}(x)$ and $\phi_{\leftarrow}(x)$ were constructed above. Requiring that this form of ϕ_E satisfies the Bloch periodicity conditions at $x = \pm L/2$ then gives an equation relating q and E (deriving this is good practice, but not required),

$$\boxed{\cos(qL) = \frac{t^2 - r^2}{2t} e^{ikL} + \frac{1}{2t} e^{-ikL} \ .}$$

Where t and r are the transmission and reflection amplitudes of the single potential barrier constructed above.

(a) Show that this condition on q and E, together with the definition of the scattering phase given above, leads to

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

Aside: The band structure is thus **completely determined** *by the transmission probability and the phase shift! This is another reason scattering information is so valuable – it encodes a great deal more than just "how likely is it i'll tunnel through this wall?"*

(b) For $V(x)$ a generic potential, explain why there are no solutions to the equation derived in part (a) in the regions around $kL - \varphi = n\pi$, for any integer n. These are the gaps. What role does the scattering phase play in the band structure?

(c) Suppose the barriers in $V(x)$ are very *weak*. What does this imply about T, R and φ? Show that, in this limit, the energy gaps are very narrow, with the width of the gap around $kL - \varphi = n\pi$ given, approximately, by,

$$\Delta E_{gap} \propto \sqrt{R}$$

Sketch $E(q)$ in this limit.

(d) Supposed the barriers in $V(x)$ are very *strong*. What does this imply about T, R and φ? Show that, in this limit, the allowed energy bands are very narrow, with

$$\Delta E_{band} \propto \sqrt{T}$$

Where are the allowed bands centered in this limit? Sketch $E(q)$ in this limit.

(e) For $V(x)$ a delta-function barrier with $g_o > 0$, use previous results (*see Problem 5 in Solution Set 7 where we studied transmission for a delta-function well of strength* $-V_o$) to show[1] that,

$$\cot(\varphi) = \frac{2kL}{g_o} \qquad T = \cos^2(\varphi)$$

Use this result and your result from part (a) to reproduce the result derived in lecture for the periodic array of delta-function barriers,

$$\cos(qL) = \cos(kL) + \frac{g_o}{2kL}\sin(kL) \ .$$

Verify that the results you found for a general potential in parts (b-d) obtain for this specific potential by making a precise plot (via Mathematica, Matlab, etc.) of $E(q)$ in the limit $g_o \ll 1$ and $g_o \gg 1$.

(f) Now consider a lattice of *attractive* delta functions with $g_o < 0$. Again plot $E(q)$ for large and small magnitude of g_o. What has happened to the single bound state of the isolated attractive delta function?

[1] The following trig identities are useful in this calculation:

$$\cos\left(\cot^{-1}(b)\right) = \frac{b}{\sqrt{1+b^2}} \qquad \sin\left(\cot^{-1}(b)\right) = \frac{1}{\sqrt{1+b^2}} \qquad \cos(a+b) = \cos(a)\cos(b) - \sin(a)\sin(b)$$

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

Aside: The appearance of gaps in the spectrum of energy eigenvalues is a striking feature of the periodic potential. As we have seen, the widths of these gaps decrease to zero as the strength of the barriers between wells vanishes. Thus, the state at the top of one band and the state at the bottom of the next band become degenerate *as the potential is turned off. Conversely, then, the periodic potential must* break *a degeneracy among two free particle states, with one state becoming higher energy than the other as the potential is turned on. In this problem we will explore this process by studying the states at band edges.*

Consider the lattice of delta functions studied in lecture, $V = \sum \frac{\hbar^2}{2m} \frac{g_o}{L} \delta(x - nL)$, and focus on the states at the edges of the bands with crystal momentum $qL = N\pi$.

(a) The states at the edges of the allowed energy bands have $qL = N\pi$. Why?

(b) Let's start by thinking through the qualitative shape of the wavefunctions at the band edges, $qL = N\pi$. If we could turn off the potential, we would find two degenerate free-particle states, $\sin(qx)$ and $\cos(qx)$, both of which are periodic with period $\frac{2L}{N}$. Now imagine gradually turning on the potential. What does the delta function potential do to our two degenerate wavefunctions? Make a qualitative sketch of the resulting wavefunctions. Which of the two states becomes the top of a band, and which becomes the bottom of a band? What can you say about the higher-energy state in the limit $g_o \to \infty$?

(c) Now let's check this picture. To begin, identify the boundary conditions which ϕ_E and ϕ_E must satisfy at $x = 0$. What periodicity condition must ϕ_E satisfy?

(d) In the region $0 < x < L$, the potential is constant so ϕ_E can be written as a solution to the free particle equation, $\phi_E(x) = A\sin(kx + \theta)$, where $E = \frac{\hbar^2 k^2}{2m}$ and θ is a phase. Express the boundary conditions on ϕ_E as conditions on k and θ.

(e) Show that half of solutions to these conditions are standing waves with $kL = N\pi$ and $\theta = 0$. Do these states appear at the top or bottom of their bands?

(f) Show that the other half of the solutions satisfy:

$$\tan\left(\frac{kL}{2}\right) = -\frac{2kL}{g_o} \ ,$$

when $qL = (2M+1)\pi$ and

$$\cot\left(\frac{kL}{2}\right) = \frac{2kL}{g_o} \ ,$$

when $qL = 2M\pi$. Do these states appear at the top or the bottom of their bands?

(g) What happens to the states at the band edges as you make the barriers strong, $g_o \to \infty$? What happens to the width of the gap? Does this make sense?

(h) What happens to the states at the band edges as you make the barriers weak, $g_o \to 0$? What happens to the width of the gap? Does this make sense?