QUANTUM MECHANICS I

PHYS 516

Final Examination
Distributed: March 8, 2010
Due: March 15, 2010, 11:00 am

1. Systematics of Level Crossings: A one-dimensional bimodal potential is $V(x) = \frac{1}{4}x^4 + ax^2 + bx$. Use $a = -2$ and b as assigned below.

a. Choose a suitable interval $[-L, +L]$ on the line and discretize this problem.

b. Diagonalize the appropriate matrices and list the six lowest eigenvalues.

c. Plot the two lowest eigenvectors.

d. Plot the probability distributions associated with the two lowest eigenvectors.

Finlay	Groener	Jones	Moorman	O'Brien	E. Smith	M. Smith
-2	-1	$-\frac{1}{2}$	0	$\frac{1}{2}$	$+1$	$+2$

2. Simple Lattice: N atoms of mass m are connected to each other by springs of spring constant k, subject to periodic boundary conditions. Assume only nearest neighbor interactions.

a. Compute the normal modes.

b. Plot the energy dispersion relation.

3. Next Nearest Neighbor Interactions: The lattice described above now undergoes nearest neighbor interactions with springs of spring constant k and experiences next nearest neighbor interactions with springs with spring constant κ.

a. Write down the appropriate eigenvalue equation.

b. Describe the normal modes.

c. Plot the dispersion relation assuming $1 + \frac{4\kappa}{k} = 0$. Provide appropriate remarks about this dispersion relation.

d. If κ is sufficiently large does the dispersion relation have a maximum inside the band edge? If so, how large must κ be to see this effect?

4. Vacuum Force: A linear lattice consists of N atoms of mass m connected (nearest neighbor) by springs with spring constant k, with the two end atoms connected to brick walls (fixed boundary conditions).

a. Compute the ground state energy

$$E_g(N) = \sum_{j=1}^{N} \frac{1}{2}\hbar\omega(j)$$

b. Plot $E_g(N)$ as a function of N for $2 \leq N \leq 100$. Set $\hbar\omega_0 = 1$.

c. Set $N = 100$. Nail down the kth mass in its equilibrium position. How much energy does this cost?

d. Plot this energy cost as a function of k, $1 \leq k \leq 99$.

e. Is there a force on the nail? How big and which direction?

5. Temperature-Dependent Fluctuation Forces: The lattice described in Problem #4 is now in thermal equilibrium with its surroundings at temperature T.

a. Show that the mean energy in a mode with angular frequency ω is

$$\langle E \rangle = \left(\langle n \rangle + \frac{1}{2} \right) \hbar\omega \qquad \text{where} \qquad \langle n \rangle = \frac{1}{e^{\beta\hbar\omega} - 1}$$

b. Compute the mean energy in the lattice with $N = 100$ atoms for $\beta\hbar\omega_0 = 0.1, 0.25, 0.5, 1.0$. Recall that $\omega(j) = 2\omega_0 |\sin((j\pi/2)/(N+1))|$.

c. How much energy does it take to fix the $25th$ mass in place for $\beta\hbar\omega_0 = 0.25$?

d. Estimate the force on the nail under these conditions.

6. Two Atoms per Unit Cell: A one-dimensional lattice with N cells has two atoms of masses m and M per unit cell. The atoms within a unit cell are connected by a spring with spring constant K. Adjacent unit cells are connected by springs with constant k. Assume periodic boundary conditions.

a. Qualitatively describe the normal modes.

b. Assume $M = 2m$ and $K = 3k$ and set $k/m = \omega_0^2$. Compute and plot the dispersion relations. Clearly specify the acoustic and the optical branches.

c. Describe both qualitatively and quantitatively the two normal modes within a unit cell for normal mode with index j.

7. "... the Usual Suspects": Bob and Carol and Ted and Alice are confined to the 9^{th} circle (a quantum mechanics class). The presiding devil assigns the following problem on the final exam: "A one-dimensional harmonic lattice has 3 atoms/unit cell, N cells, and periodic boundary conditions. The atoms have masses m_1, m_2, m_3 and are connected by springs with constants k_{12} and k_{23} within a cell, and by a weaker spring with constant k_{31} across unit cells. Assume $m_1 = 5, m_2 = 7, m_3 = 3$, also $k_{12} = 6, k_{23} = 4$, and finally $k_{31} = 1$. Plot the dispersion relations for the three branches."

Carol is a very assiduous student. She performs the requested computations and plots the way she was taught. Bob, on the other hand, is incredibly lazy and is always looking for the Quick and Dirty shortcut.

a. Repeat Carol's computations.

b. Bob's hairbrained idea is to follow Carol's computation up to the creation of a 3×3 matrix depending on the phase shift $\epsilon = e^{2\pi ij/N}$. Rather than finding the eigenvalues for all allowed complex values of the phase shift, Bob solves this for only the two values $\epsilon = +1$ at the band center and $\epsilon = -1$ at the band edges ("this ought to be enough" (?)). Do this.

c. Bob then fits trigonometric functions through these points. Do this.

d. Then Bob takes the square roots of these fitted curves (why?). Do this also.

e. How good/bad is this "fit" compared to Carol's?

f. Ted and Alice (dispassionate observers snickering from the sidelines) point out to Bob that maybe fitting trig functions and taking square roots don't commute (after all, this *is* a quantum course). Perhaps if he took square roots of the two sets of three eigenvalues, *and then* fitted the appropriate trig functions, he could do better. Are they right?