Physics Department

8.231, Physics of Solids I

Due in Ses #16

Problem Set #3

Problem 1: A Square Lattice (Similar to problem 4.1 in the 6th edition of Kittel but absent from the 7th edition)

Consider the vibrations of a planar square lattice of lattice constant a. There is only one atom of mass M in each primitive unit cell and it is restricted to motions perpendicular to the plane (transverse motion). We will assume only nearest neighbor interactions, for which the force constant is C. Let $u_{l,m}$ denote the transverse displacement of the atom in the lth column and the mth row.

a) Show that the equation of motion is

$$M \frac{d^2 u_{lm}}{dt^2} = C \left[\left(u_{l+1,m} + u_{l-1,m} - 2u_{lm} \right) + \left(u_{l,m+1} + u_{l,m-1} - 2u_{lm} \right) \right].$$

b) Show that the dispersion relation is found from the expression

$$M\omega^2 = 2C(2 - \cos k_x a - \cos k_y a).$$

c) Find the first Brillouin zone. Sketch the dispersion curve, ω verses k along the \hat{x} direction, the direction where $k_x = k_y$, and along a straight line path from $(\frac{\pi}{a}, 0)$ to $(\frac{\pi}{a}, \frac{\pi}{a})$.

d) Show that the dispersion curve is isotropic for small k, and find the limiting value of the group velocity as $k\rightarrow 0$, that is, the sound velocity in the lattice.

Problem 2: Atomic Displacements in the Diatomic Linear Chain

Do problem 3 (4) at the end of chapter 4 of 7^{th} (6th) edition of Kittel.

Problem 3: A Different Diatomic Chain

Do problem 5 (6) at the end of chapter 4 of 7^{th} (6th) edition of Kittel.

It is often said that phonons are sound waves in a crystal. This is not strictly true. In fact, a sound wave is a coherent state of the harmonic oscillator which is associated with a particular phonon. In a similar way, the microwave radiation from a klystron or the optical radiation from a laser well above threshold are coherent states of the electromagnetic field. The following three questions are designed to introduce you to (or remind you of) the coherent state of a harmonic oscillator.

Problem 4: Time-Dependent Wavefunctions

An arbitrary time-dependent wavefunction $\Psi(x,t)$ can be written in terms of the time-independent energy eigenfunctions $\psi_n(x)$ as follows:

$$\Psi(\mathbf{x},t) = \sum_{n=0}^{\infty} c_n e^{-i\frac{E_n t}{\hbar}} \psi_n(\mathbf{x}).$$

a) Assuming the ψ_n form an orthonormal complete set, $\int_{-\infty}^{\infty} \psi_m^*(x)\psi_n(x) dx = \delta_{mn}$, find the coefficients c_n in terms of the wavefunction at t=0, $\Psi(x,t=0)$.

b) In the case of a simple harmonic oscillator of frequency ω , show that, with the possible exception of a factor of -1, $\Psi(x,t)$ is periodic with a period $T = 2\pi/\omega$.

Problem 5: Consequences of Spatial Localization for a Harmonic Oscillator

For a harmonic oscillator we will show that if $\Psi(x,t=0) = \delta(x-x_0)$, then $\Psi(x,t=T/4)$ is a plane wave.

a) Expand $\Psi(x,t)$ in terms of the energy eigenfunctions $\psi_n(x)$. Find a expression for the expansion coefficients, c_n in terms of the $\psi_n(x_0)$. Write down the expression for $\Psi(x,t=T/4)$ as an infinite sum over the energy eigenstates.

b) The formal expression found in a) for $\Psi(x,t=T/4)$ does not appear at all like a plane wave. However, plane waves are eigenstates of the momentum operator, $-i\hbar\frac{\partial}{\partial x}$. Apply this operator to $\Psi(x,t=T/4)$. Use the recursion relations below to express $\frac{\partial \Psi_n(x)}{\partial x}$ in terms of Ψ_{n+1} and Ψ_{n-1} . Rearrange the resulting sum so that each $\Psi_{n'}(x)$ appears only once with a coefficient containing both $\Psi_{n'-1}(x_0)$ and

 $\Psi_{n'+1}(x_o)$. Use the recursion relations again to consolidate these terms in such a way that $\Psi(x,t=T/4)$ is retrieved. What is the particle's momentum at t=T/4?

The energy eigenstates of a harmonic oscillator obey the recursion relations

$$\left\lfloor \frac{x}{a} + a \frac{d}{dx} \right\rfloor \psi_n(x) = \sqrt{2} \sqrt{n} \psi_{n-1}(x)$$

$$\left[\frac{x}{a} - a\frac{d}{dx}\right]\psi_n(x) = \sqrt{2}\sqrt{n+1}\psi_{n+1}(x)$$

where $a \equiv \sqrt{k/m\omega}$.

Problem 6: The Coherent State

The probability density associated with an energy eigenfunction is independent of time. In particular, it does not oscillate back and forth in space. The quantum state which most closely approximates the classical behavior of a harmonic oscillator, $V(x) = \frac{1}{2} m \omega^2 x^2$, is called the 'coherent state'. It is not an eigenstate of energy, position, or momentum.

$$\Psi(\mathbf{x},\mathbf{t}) = \left(\frac{1}{2\pi x_o^2}\right)^{\frac{1}{4}} \exp\left[-\frac{\mathrm{i}\omega t}{2} - \frac{\mathrm{i}}{2x_o^2}\left(2\alpha x_o \sin\omega t - \alpha^2 x_o^2 \sin2\omega t\right) - \left(\frac{x - 2\alpha x_o \cos\omega t}{2x_o}\right)^2\right]$$

where $x_0 \equiv (\cancel{b}2m\omega)^{\frac{1}{2}}$ and α is a dimensionless constant.

a) Find and sketch the time-dependent probability of finding the particle at x.

b) Show that $\Psi(x,t)$ satisfies the time-dependent Schroedinger equation. (This is not conceptually difficult. It just requires care and patience.)

You may be interested in some other properties of the coherent state. The probability that a measurement of the energy will give the nth energy eigenvalue, $k\omega(n+\frac{1}{2})$, is a Poisson distribution with mean value $\langle n \rangle = \alpha^2$. The coherent state is an eigenfunction of the lowering operator with eigenvalue $\alpha e^{-i\omega t}$.