3.23 Electrical, Optical, and Magnetic Properties of Materials
Fall 2007

Homework # 4

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Homework is due on Wednesday October 10th, 5pm

1 Nodal surfaces in the hydrogen atom

Draw the radial component of the 3s, 3p, and 3d orbitals for the hydrogen atom. For each of these orbitals, draw or describe the nodal surfaces and explain which ones are due to the radial component of the wavefunction, and which to the angular component.

2 Acoustic phonons in a 2D square lattice

In this problem we would like to study the dynamics of a 2 dimensional square lattice. To do this we will use the quadratic approximation to express the potential energy of the crystal. Atomic positions at equilibrium are represented by the following vectors:

$$\vec{R}_{uv} = a(u\vec{e}_x + v\vec{e}_y)$$

where a is the lattice spacing. Instantaneous atomic displacements with respect to their equilibrium position are represented by the following vectors:

$$\vec{\tau}_{uv} = x_{uv}\vec{e}_x + y_{uv}\vec{e}_y$$

where u and v are integers.

In a 2D square lattice, each atom (u, v) has 4 nearest neighbours: $(u-1, v)$, $(u+1, v)$, $(u, v-1)$ and $(u, v+1)$. In our model we will consider that each bond between two nearest neighbours has a certain energy. This energy is divided into two contributions. The first one is a **compression/elongation contribution** arising only when atoms are moving in the same direction which is the bond direction. We model this by a spring of constant k. The second contribution is a **shearing contribution** arising only when one of the atom moves perpendicular to the other. We model this by a spring of constant g. The total potential energy of the crystal is a sum over an infinite number of pairs of atoms, but the only ones where the atomic displacement of atom (u, v) appear are the following:

$$V(..., x_{uv}, y_{uv}, ...) = ... +$$
$$\left\{\tfrac{1}{2}k(x_{u+1v} - x_{uv})^2 + \tfrac{1}{2}k(x_{uv} - x_{u-1v})^2 + \tfrac{1}{2}k(y_{uv+1} - y_{uv})^2 + \tfrac{1}{2}k(y_{uv} - y_{uv-1})^2\right\}+$$
$$\left\{\tfrac{1}{2}g(x_{uv+1} - x_{uv})^2 + \tfrac{1}{2}g(x_{uv} - x_{uv-1})^2 + \tfrac{1}{2}g(y_{u+1v} - y_{uv})^2 + \tfrac{1}{2}g(y_{uv} - y_{u-1v})^2\right\}+$$
$$...$$

The first four terms are the "compression/elongation" terms and the last four ones are the "shearing" terms. For example if one looks at $\frac{1}{2}g(x_{uv} - x_{uv-1})^2$, one sees that when atoms $(u, v-1)$ and (u, v) are displaced by respectively x_{uv-1} and x_{uv} in the x direction, then the relative displacement between the two atoms is $x_{uv} - x_{uv-1}$. And since this relative displacement is orthogonal to the bond direction (which is in the y direction) then a shearing energy of $\frac{1}{2}g(x_{uv} - x_{uv-1})^2$ is associated with it.

1) Write down Newton's equations for atom (u, v) given the expression for the total energy of the lattice given above. The atoms have the same mass denoted by m.

2) By using the **ansatz**:

$$\vec{r}_{uv} = (x_0\vec{e}_x + y_0\vec{e}_y)e^{i(k_x ua + k_y va - \omega t)}$$

transform Newton's equations into a 2 dimensional linear system of equations.

3) Find the dispersion relations $\omega(k_x, k_y)$. Define the first Brillouin zone for this crystal, i.e the smallest k-space unit cell that uniquely defines all the possible phonon frequencies $\omega(k_x, k_y)$.

3 Nuclear Magnetic Resonance

In NMR experiments one can actually image a body by looking at resonance peaks in the radio frequency domain corresponding to photon emission as a response to a previous magnetic exitation. In this problem we would like to focus on the physics of this resonance and find a quantum description for it. This will be an occasion for us to solve the time-dependant Schrodinger equation.

The principle of an NMR experiment is to look at the phenomenon of nuclear spin flip. To induce such a flip one uses a big homogenous magnetic field in the z direction and a small magnetic field rotating in the xy plane. Nuclei (and electrons) are like little magnets, they carry an intrinsic magnetic moment which has the property to be **proportional** to the spin, i.e $\vec{\mu} = \gamma\vec{\hat{S}}$. The total energy of a magnet in a magnetic field $\vec{B}$ reduces to the magnetic interaction of the magnet with the field:

$$E_{\text{tot}} = -\vec{\mu}.\vec{B} = -\gamma\vec{\hat{S}}.\vec{B}$$

One describes the quantum state of the magnet by a 2 dimensional vector $|\psi(t)\rangle = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix}$, where $a(t)$ and $b(t)$ are time dependant complex numbers. This description is nothing but the description of the spin quantum state of a spin one-half particle like the electron or the proton. Indeed since the magnetic moment is proportional to the spin, what we are actually looking at is the dynamics of the spin induced by the magnetic field $\vec{B}$.

1) In homework two we saw what the y projection of the spin operator was. Now we need the entire description of the spin operator. Here it is:

$$\vec{\hat{S}} = \begin{pmatrix} \hat{S}_x \\ \hat{S}_y \\ \hat{S}_z \end{pmatrix} = \hat{S}_x\vec{e}_x + \hat{S}_y\vec{e}_y + \hat{S}_z\vec{e}_z$$

The projections are operators themselves and the expression for those operators in the orthonormal basis of the eigenvectors of $\hat{S}_z$, denoted by $\{|+\rangle, |-\rangle\}$, is:

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

From the expression for the spin operator and the total energy of the magnet in a $\vec{B}$ field, write down the time-dependant Schrodinger equation for the spin state $|\psi\rangle = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix}$. The magnetic field consists of the superposition of a homogeneous magnetic field in the z direction $\vec{B}_0 = B_0\vec{e}_z$ and a rotating field $\vec{B}_1 = B_1(\cos(\omega_1 t)\vec{e}_x + \sin(\omega_1 t)\vec{e}_y)$ in the xy plane.

2) In order to simplify the resolution of this equation in $a(t)$ and $b(t)$, we will use the following ansatz for $|\psi(t)\rangle$:

$$|\psi(t)\rangle = \begin{pmatrix} c(t)e^{i\frac{\gamma B_0 t}{2}} \\ d(t)e^{-i\frac{\gamma B_0 t}{2}} \end{pmatrix}$$

Using this ansatz re-write the Schrodinger equation in terms of $c(t)$ and $d(t)$. To do this, express the left-hand side of the Schrodinger equation $i\hbar\frac{d|\psi(t)\rangle}{dt}$ in terms of $c(t)$ and $d(t)$. Then express the right-hand side by replacing $a(t)$ and $b(t)$ by respectively $c(t)e^{i\frac{\gamma B_0 t}{2}}$ and $d(t)e^{-i\frac{\gamma B_0 t}{2}}$. Simplify as much as you can the terms remembering that $\cos(x) + i\sin(x) = e^{ix}$ and $\cos(x) - i\sin(x) = e^{-ix}$. The final equations in $c(t)$ and $d(t)$ should be simple.

3) The solution for those equations, given that at $t = 0$ we consider that $|\psi(0)\rangle = |+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, are:

$$\begin{pmatrix} c(t) \\ d(t) \end{pmatrix} = \begin{pmatrix} \frac{1}{\omega_- - \omega_+}(\omega_- e^{i\omega_+ t} - \omega_+ e^{i\omega_- t}) \\ \frac{2e^{-i(\omega_+ + \omega_-)t}}{\gamma B_1(\omega_- - \omega_+)}\omega_+\omega_-(e^{i\omega_+ t} - e^{i\omega_- t}) \end{pmatrix}$$

where $\omega_\pm = -\frac{1}{2}(\gamma B_0 + \omega_1 \pm \sqrt{(\gamma B_0 + \omega_1)^2 + (\gamma B_1)^2})$. Given this, write down the quantum state of the system at any time t.

4) What we are interested in is the probability that at time t the system has "flipped" to a spin down state from the spin up state at time $t = 0$. Given the full expression of $|\psi(t)\rangle$ of question 3), calculate this transition probability $P_{|+\rangle\to|-\rangle}(t)$ to measure the system in a "spin down" state at time t. Give your answer in terms of γ, B_0, B_1, ω_1 and t.

5) From question 4), calculate the maximum value for the transition probability. Plot the maximum probability as a function of ω_1 considering that ω_1 can take positive **and** negative values (this relates to the fact that $\vec{B}_1$ can rotate clockwise or anti-clockwise in the xy plane). What is the width at half maximum $\Delta\omega$?

6) What is the limit of $\Delta\omega$ when the amplitude of the rotating magnetic field B_1 is going to zero? What can you conclude from that?

discussion: In an hospital, one can use an NMR system to image the brain of a patient for example. To do this, superconducting coils are used to create an inhomogeneous $\vec{B}_0$ field. Then a rotating field $\vec{B}_1$ is created with a definite frequency ω_1. Now since the resonance frequency is given by $\gamma||\vec{B}_0||$ and the sharpness of the resonance is given by $2\gamma B_1$, one can see that if B_1 is really small, then only areas of the brain where the local field $\vec{B}_0$ is such that $\gamma||\vec{B}_0|| = \omega_1$ will absorb and emit radio photons. If we somehow have a way to determine from what points in space the emitted photons originated, then we have a device that is capable of precisely imaging areas of the brain that have the same chemical and magnetic environment.