MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Physics Department

8.231, Physics of Solids I Due on Wed., Oct 11.

Problem set #4

1. Let $\psi_x^p = f(r)x$ be the normalized wave function that describes an atomic p_x orbital and let $\psi^s = g(r)$ be the normalized wave function that describes an atomic s orbital. We assume that $g(r)$ and $f(r)$ are positive for large r. We can define a more general atomic p orbital as

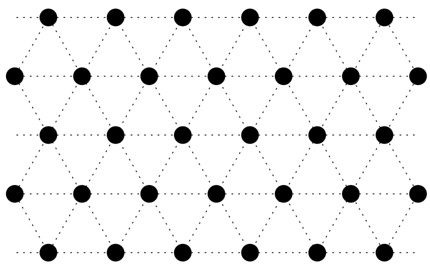
$$\psi_{\boldsymbol{n}}^p = f(r)\boldsymbol{r} \cdot \boldsymbol{n}$$

where $\boldsymbol{n}$ is a unit vector that can point to any direction.

   (a) Calculate the inner product between two p orbitals $\langle \psi_{\boldsymbol{n}_2}^p | \psi_{\boldsymbol{n}_1}^p \rangle$.

   (b) Use ψ^s, ψ_x^p, and ψ_y^p to construct three sp mixed orbitals that point to three directions $\boldsymbol{n}_1$, $\boldsymbol{n}_2$, and $\boldsymbol{n}_3$ in the x-y plane. The angles between $\boldsymbol{n}_1$, $\boldsymbol{n}_2$, and $\boldsymbol{n}_3$ are all 120°. Note that the three sp mixed orbitals are described by three orthonormal wave functions.

2. (40 pts) Beads of mass m are connected by springs of length $a = 1$ and form a triangular lattice (see the figure below).



The spring constants of the springs are all given by C.

   (a) Find the fundamental translation vectors $(\boldsymbol{a}_1, \boldsymbol{a}_2)$ of the triangular lattice. Find the fundamental translation vectors $(\boldsymbol{b}_1, \boldsymbol{b}_2)$ of the reciprocal lattice. We may choose the Wigner-Seitz unit cell of the reciprocal lattice as the Brillouin zone. Draw such a Brillouin zone.

   (b) The total potential energy of the deformed lattice is given by

$$U_{\text{tot}} = \frac{1}{2} \sum_{\boldsymbol{ij}} \vec{u}_{\boldsymbol{i}} C_{\boldsymbol{ij}} \vec{u}_{\boldsymbol{j}}$$

   where $\boldsymbol{i}$ is the location of a point in the triangular lattice and $\vec{u}_{\boldsymbol{i}}$ is the displacement of the bead at the location $\boldsymbol{i}$. Calculate the two by two matrix $C_{\boldsymbol{ij}}$.

   (c) Calculate the dispersion relation $\omega_{\boldsymbol{k}}$ of the two branches of sound waves. (Hint: you may want to introduce (k_1, k_2) through $\boldsymbol{k} = k_1 \frac{\boldsymbol{b}_1}{2\pi} + k_2 \frac{\boldsymbol{b}_2}{2\pi}$ and express $\omega_{\boldsymbol{k}}$ as a function of k_1 and k_2.)

   (d) Plot the dispersion relations along the following lines $\boldsymbol{k} = 0 \to \frac{1}{2}\boldsymbol{b}_1 \to \frac{1}{2}(\boldsymbol{b}_1 + \boldsymbol{b}_2) \to 0$. Mark those lines in your Brillouin zone. (This is also the good time to plot the dispersion relation along several directions that are related by symmetry to check your result.)