PHY460: Problem Set #3 Due: Friday 10/20 by 5pm in Yellow PHY460 homework box between Loomis and MRL on 2nd Floor

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1. Free electron energies on the square lattice in the empty lattice approximation

   (a) Show for a simple square lattice (two dimensions) that the kinetic energy of a free electron at a corner of the (first) Brillouin zone is higher than that of an electron at the midpoint of a side face of the Brillouin zone by a factor of 2.

   (b) What is the corresponding factor for a simple cubic lattice (i.e., in three dimensions)?

2. The primitive translation vectors of the 3D hexagonal/honeycomb lattice may be taken as

$$\mathbf{a}_1 = (\sqrt{3}a/2)\hat{x} + (a/2)\hat{y}; \quad \mathbf{a}_2 = -(\sqrt{3}a/2)\hat{x} + (a/2)\hat{y}; \quad \mathbf{a}_3 = c\hat{z}. \tag{1}$$

   (a) Show that the volume of the primitive cell is $(3^{1/2}/2)a^2c$.

   (b) Show that the primitive basis vectors of the reciprocal lattice are

$$\mathbf{b}_1 = (2\pi/\sqrt{3}a)\hat{x} + (2\pi/a)\hat{y}; \quad \mathbf{b}_2 = -(2\pi/\sqrt{3}a)\hat{x} + (2\pi/a)\hat{y}; \quad \mathbf{b}_3 = (2\pi/c)\hat{z}. \tag{2}$$

   Show that this implies that the lattice is its own reciprocal, except for a rotation and re-scaling of axes.

   (c) Describe and sketch the (first) Brillouin zone of the hexagonal space lattice.

3. For the primitive lattice in the previous problem draw (at least) a 5×5 set of unit cells/lattice points in the $\vec{a}_1$ and $\vec{a}_2$ plane, *i.e.* draw lattice points that are constructed as $\vec{R} = n\vec{a}_1 + m\vec{a}_2$. Draw lines representing the 2d Miller indices (10), (01), (11), (21), (12), (41)

4. Show that the generically in 3d the volume of the (first) Brillouin zone is $(2\pi)^3/V_c$, where V_c is the volume of a real-space crystal primitive cell. Hint: The volume of a Brillouin zone is equal to the volume of the primitive parallelepiped in reciprocal space. Recall the vector identity $(\mathbf{c} \times \mathbf{a}) \times (\mathbf{a} \times \mathbf{b}) = (\mathbf{c} \cdot (\mathbf{a} \times \mathbf{b}))\mathbf{a}$.

5. Consider a periodic potential $V(x, y) = \sin(2\pi x/a) + \sin(4\pi y/a)$.

   (a) Write down a set of primitive lattice vectors $\vec{a}_1, \vec{a}_2$ that define the period of this potential.

   (b) Fourier expand $V(x, y) = \sum_{\vec{G}} V_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$ by determining the set $\vec{G}$ and the coefficients $V_{\vec{G}}$.

   (c) Show that the $\vec{R} \cdot \vec{G} = 2\pi q$ for an integer q where $\vec{R} = n\vec{a}_1 + m\vec{a}_2$.

   (d) Repeat steps (a) through (c) for the potential $V(x, y) = \sin(2\pi(x + y)/a) + \cos(2\pi(x - 2y)/a)$.

   (e) For both sets of potentials convert the continuous periodic potential into a discrete set of lattice points (draw a subset of these points which illustrates the lattice structure). This can be done by choosing a point somewhere inside a cell of each periodic potential and translating that point by the respective $\vec{a}_1, \vec{a}_2$. How does the resulting lattice change if we pick a different starting point within a cell of the periodic potential?

6. Using the $\vec{G}$ derived in the previous problem

   (a) Write down an explicit form for the Bloch functions for both potentials and show that they are periodic when translated by a lattice translations $\vec{R} = n\vec{a}_1 + m\vec{a}_2$ for all integers n, m.

   (b) Multiply each Bloch function by a suitable plane wave so that it represents an eigenstate of $H = \frac{p^2}{2m} + V(x, y)$.

   (c) Determine the allowed range for the wave vector $\vec{q}$ entering the plane wave piece and draw the 2d Brillouin zone (which contains all unique values of q) for each potential.

   (d) Find translation operators $T(\vec{d}) = e^{i\vec{d}\cdot\vec{p}/\hbar}$ that commute with the Hamiltonian, *i.e.* determine the smallest allowed values of the vector $\vec{d}$ such that $T(\vec{d})$ commutes with $H = \frac{p^2}{2m} + V(x, y)$ for the two choices of $V(x, y)$. Show explicitly that $[T(\vec{d}), H] = 0$. Show that the eigenstates determined in part (c) are eigenstates of these translation operators.