PHY-715: Solid State Physics, UMass Amherst, Problem Set #2

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Due: Friday, March 12.

I. IMPURITY IN A CHAIN

Consider a tight-binding chain where one of the atoms in the chain (say, at site $n = 0$) is an impurity such that it has an atomic orbital energy which differs by an amount $\Delta\epsilon$ from all the other atomic orbital energies:

$$H = -t \sum_n \left(|n+1\rangle\langle n| + \text{h.c.} \right) + \epsilon_0 \sum_n |n\rangle\langle n| + \Delta\epsilon \, |0\rangle\langle 0| \, . \tag{1}$$

1. Look for a solution of the form $|\phi\rangle = \sum_n \phi_n |n\rangle$, with $\phi_n = C\mathrm{e}^{-qa|n|}$ (localized wavefunction), with $q > 0$ real, and a the lattice spacing. Show that there is a localized eigenstate for any negative $\Delta\epsilon$, and find the corresponding energy.

2. Let us now investigate how this impurity scatters a plane wave incoming from the left with unit amplitude. We look for solutions of the form $\phi_n = \mathrm{e}^{-ikan} + R\mathrm{e}^{ikan}$ for $n < 0$, and $\phi_n = T\mathrm{e}^{-ikan}$ for $n \geq 0$. Determine the transmission T and reflection R amplitudes as a function of k.

II. DIATOMIC TIGHT BINDING CHAIN

Consider a tight-binding chain with two alternating types of atoms A and B, with different onsite energies ϵ_A and ϵ_B, while the hopping matrix elements are $-t$. The two neighbors of each atom A are of type B, and vice and versa, so the chain has the structure $\cdots - A - B - A - B - A - \ldots$ The Hamiltonian reads

$$H = -t \sum_n \left(|n, B\rangle\langle n, A| + |n+1, A\rangle\langle n, B| + \text{h.c.} \right) + \epsilon_A \sum_n |n, A\rangle\langle n, A| + \epsilon_B \sum_n |n, B\rangle\langle n, B| \, . \tag{2}$$

Calculate the band structure (dispersion relation) of this model, you should find two bands. Plot the dispersion relation in both the reduced ($k \in [-\pi/a, \pi/a]$) and extended ($k \in [-\pi/(a/2), \pi/(a/2)]$) zone schemes. Make sure you recover the result derived in class if $\epsilon_A = \epsilon_B$. Assume that both atoms are monovalent ($Z = 1$), is the system a metal or an insulator?

III. GRAPHENE

Graphene is a two-dimensional lattice of carbon atoms, arranged in a honeycomb lattice. Note that the honeycomb lattice is not a Bravais lattice, but instead is best thought as two triangular sublattices.

1. Find the expression of the primitive lattice vectors $\vec{a}_1$ and $\vec{a}_2$ shown in Fig. 1 (next page), in terms of the inter-atom distance a. Describe the structure of the reciprocal lattice.

2. Let's call A the atoms in red, corresponding to the triangular lattice Λ, and B the atoms on the sublattice shifted by $\vec{d} = (-a, 0)$. We use $|\vec{r}, A\rangle = |\vec{r}\rangle$ and $|\vec{r}, B\rangle = |\, \vec{r} + \vec{d}\, \rangle$ to label those atoms. The Hamiltonian is

$$H = -t \sum_{\vec{r} \in \Lambda} \sum_{\vec{n} = \vec{0}, \vec{a}_1, \vec{a}_2} |\vec{r}, A\rangle\langle \vec{r} + \vec{n}, B| + \text{h.c.}, \tag{3}$$

   where the sum over $\vec{n} = \vec{0}, \vec{a}_1, \vec{a}_2$ corresponds to the 3 neighbors of each A atoms. Look for plane wave solutions $|\psi_{\vec{k}}\rangle = \frac{1}{\sqrt{2N}} \sum_{\vec{r} \in \Lambda} \mathrm{e}^{i\vec{k}\cdot\vec{r}} \left(C_A |\vec{r}, A\rangle + C_B |\vec{r}, B\rangle \right)$, and find the corresponding energies $\epsilon_{\vec{k}}$. (You should find two bands)

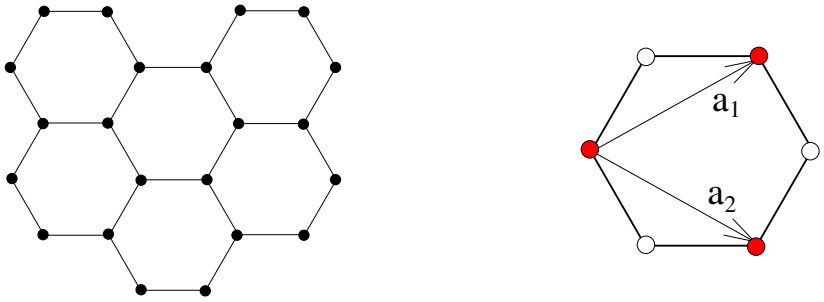

FIG. 1: Honeycomb lattice, and primitive vectors.