Physics 152B/232 **Spring 2025**

Problem Set 2

Problem 1

Consider a one-dimensional chain of alternating atoms A and B

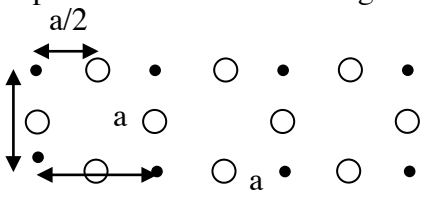
A B A B A B A B A B A B

Assuming one s-orbital per atom and only nearest neighbor Hamiltonian matrix elements and overlaps, find the tight binding band structure $\varepsilon_\nu(k)$ in terms of H_{AA}, H_{AB}, H_{BB} and S.

Ex

Problem 2

The figure shows the planes of cuprate materials that are high Tc superconductors.



The black circles are Cu atoms, the open circles are O atoms.

Assume one $d_{x^2-y^2}$ orbital for each Cu atom, and p_x and p_y orbitals for each O atom, where x and y are horizontal and vertical directions, to construct a tight binding Hamiltonian. Assume all orbitals are orthogonal to each other, and that the energy of an electron in a p orbital is lower than in the d orbital.

(a) List all the tight binding Hamiltonian parameters that you need assuming off-diagonal matrix elements only for nearest neighbor Cu-O and O-O atoms. How many are they?

(b) Construct the hamiltonian matrix $E_{nn'}(\vec{k})$ neglecting the off-diagonal O-O matrix elements for simplicity. Explain all the steps.

(c) Find an expression for the energy eigenvalues as function of k in the direction connecting the points Γ=(0,0) and D=(π/a,0) in the Brillouin zone. Same for the direction connecting the points Γ=(0,0) and X=(π/a, π/a,) in the Brillouin zone.

(d) Assume energy eigenvalues at the point Γ are -2.2eV and -3.5eV, and the highest energy eigenvalue at point D is 0.6eV. Find the values for the tight binding Hamiltonian parameters, and plot the energy bands in the directions Γ-D and Γ-X.

Problem 3

Consider a system that has n electrons, with ground state) energy E(n). We can define the effective Coulomb repulsion for two electrons of opposite spin added to this system as:

$$U_{eff} = [E(n+2) - E(n+1)] - [E(n+1) - E(n)]$$

(a) Calculate U_{eff} for the hydrogen ion H^+ assuming the wavefunction for two electrons is the product of the single electron wavefunctions for H.

(b) Same assuming the wavefunction for two electrons is the one found in HW1 Prob. 5.

(c) Find an experimental value for U_{eff} for H^+, and find the difference between it and the value found in (b).

(d) Repeat (a), (b), (c) for He^{++} and for Li^{+++}.

(e) Find an experimental value for U_{eff} for O^+.

Problem 4 [for 232 students; extra credit for 152B students]

Find the energy bands of graphene. Assume one orbital per atom of zero energy, and only matrix elements t connecting nearest neighbor atoms, at distance a apart.
Use as primitive lattice vectors:

$$\vec{a}_1 = \sqrt{3}a\hat{x} \quad ; \quad \vec{a}_2 = \frac{\sqrt{3}}{2}a(\hat{x} + \sqrt{3}\hat{y})$$

(a) What are the reciprocal lattice vectors for these primitive vectors?

(b) Find an expression for the energy bands ε_k versus $\vec{k}$.

(c) There is a point in k-space (Dirac point) where the energy goes to zero linearly as a function of the wavevector measured from that point. That point is $\vec{K} = \frac{4\pi}{3\sqrt{3}a}\hat{x}$.

Show that the energy bands found in (b) yield, for $\vec{k} = \vec{K} \pm \vec{q}$:

$\varepsilon_k = Cq$

and find the value of the constant C in terms of t and a. Show all steps in the calculations.