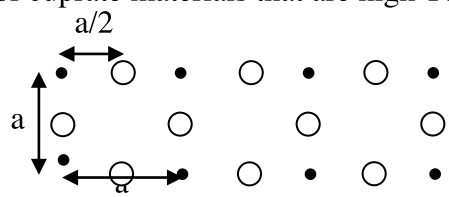
Physics 152B **Spring 2024**

Problem Set 2

Problem 1

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.

(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 -2.1eV and -3.4eV, and the highest energy eigenvalue at point D is 0.5eV. Find the values for the tight binding Hamiltonian parameters, and plot the energy bands in the directions Γ-D and Γ-X.

Problem 2

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 3

Find U_{eff} as defined in problem 2 for electrons interacting with an ion that can move, described by the Hamiltonian

$$H = \frac{-\hbar^2}{2M}\nabla_q^2 + \frac{1}{2}Kq^2 + \alpha q(c_\uparrow^+ c_\uparrow + c_\downarrow^+ c_\downarrow) + U n_\uparrow n_\downarrow$$

where q denotes the spatial position of the ion that has mass M and vibrates around its equilibrium position q=0 with frequency $\omega = \sqrt{K/M}$. The operator c_σ^+ creates an electron of spin σ in that ion, $n_\sigma = c_\sigma^+ c_\sigma$.

Problem 4

Consider a chain of N electrons and N ions described by the Hamiltonian

$$H = H_{ions} - \sum_{i,\sigma} -(t - \alpha(q_{i+1} - q_i))(c_{i,\sigma}^+ c_{i+1,\sigma} + h.c)$$

$$H_{ions} = \frac{-\hbar^2}{2M}\sum_i \nabla_{q_i}^2 + \frac{1}{2}K\sum_i (q_{i+1} - q_i)^2$$

There are equal number of electrons of each spin. Assume that because M is very large we can ignore the motion of the ions and assume the ions are at static positions q_i.

(a) Find the ground state energy assuming $q_i = 0$ for all i.

(b) Find the ground state energy assuming $q_i = (-1)^i \delta$, call it $E_g(\delta)$

(c) Find a value of δ for which $E_g(\delta) > E_g(0)$

(d) Find a value of δ for which $E_g(\delta) < E_g(0)$