Physics 152B **Spring 2024**

Problem Set 3

Problem 1

Consider the tight binding energy band for a two-dimensional square lattice with lattice spacing a and nearest neighbor hopping t.
(a) Find the effective mass of carriers when the band is almost empty and when it is almost full.
(b) Find the shape of the Fermi surfaces when the band is close to empty, when it is half-full, and when it is close to full. Make a plot of the first Brillouin zone showing the three Fermi surfaces.
(c) Find the ground state energy of the system when the band is half full.
(d) Find an expression for the density of states in energy when the band is close to empty and when it is close to full.

Problem 2

Consider a two-site Hubbard model with Hamiltonian

$$H = -t\sum_{\sigma}(c_{1\sigma}^{+}c_{2\sigma} + h.c.) + U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow})$$

where the operators $c_{i\sigma}^{+}, c_{i\sigma}$ create and destroy electrons of spin $\sigma = \uparrow$ or $\downarrow$ in an atomic orbital at site i. $n_{i\sigma} = c_{i\sigma}^{+}c_{i\sigma}$. Assume t>0 and U>0.

(a) Find the eigenstates and eigenvalues of the Hamiltonian when there is one electron in the system.
(b) Find the eigenstates and eigenvalues of the Hamiltonian when there are three electrons in the system.
(c) Find the eigenstates and eigenvalues of the Hamiltonian when there are two electrons with antiparallel spin in the system.
(d) Find the eigenstates and eigenvalues of the Hamiltonian when there are two electrons with parallel spin in the system.
(e) Show that in the limit of large U/t, the difference in energy between ferromagnetic and antiferromagnetic states (i.e. lowest energies for (d) and (c)) is proportional to t^2/U. What is the proportionality constant? Which state has lower energy?

Problem 3

(a) For the two-site Hubbard model of Problem 2, find the effective Coulomb repulsion for two electrons with antiparallel spins in this system,

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

, as a function of t and U, where E(n) is the lowest energy of the system with n electrons, and n=0. Find the limiting values of U_{eff} for U→0 and U→+infinity, and make a qualitative plot of U_{eff} versus U/t.
(b) Repeat (a) for n=2, where the two electrons when n=2 have antiparallel spins.

Problem 4

Consider the equation derived in class for the binding energy of a Cooper pair, applied to a one-dimensional Hubbard model with N sites, with the band half full. The parameter v_0 in the equation in the lecture is (-U)/N. Assume U<0, i.e. the interaction is attractive.. Find an expression for the binding energy of a Cooper pair when |U|/t<<1.

Problem 5

Consider a two-site generalized Hubbard model

$$H = -t\sum_{\sigma}(c_{1\sigma}^{+}c_{2\sigma} + h.c.) + U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}) + X\sum_{\sigma}(c_{1\sigma}^{+}c_{2\sigma} + h.c.)(n_{1,-\sigma} + n_{2,-\sigma})$$

with t>0 and X>0 and U>0.

(a) Repeat what you did in Problem 3 and find expressions for $U_{eff}(n=0)$ and $U_{eff}(n=2)$ in terms of t, U and X.

(b) Find conditions on the parameters such that U_{eff} <0, i.e. the effective interaction is attractive. Can that happen for n=0? For n=2?