Physics 152B/232 **Spring 2025**

Problem Set 3

Problem 1

Find U_{eff} as defined in problem 3 of HW 2 for electrons interacting with an ion that can move, described by the Hamiltonian

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

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 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) Same as (a) 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 $|U|/t \ll 1$.

Problem 5

Consider the Hamiltonian

$$H = -\sum_{i,j,\sigma} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + \sum_{i,j,\sigma} X_{ij} c^{+}_{i\sigma} c_{j\sigma} (n_{i,-\sigma.} + n_{j,-\sigma.}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

where $X_{ij} = \alpha t_{ij}$ and α is a positive number, and where $t_{ij} = t(R_i - R_j)$ and $t_{00} = 0$.
Write this Hamiltonian in momentum space, in terms of the operators

$c^{+}_{k\sigma} = \frac{1}{\sqrt{N}} \sum_{i} e^{ikR_i} c^{+}_{i\sigma}$ and defining $\varepsilon_k = -\frac{1}{N} \sum_{ij} e^{ik(R_j - R_i)} t_{ij} = -\sum_{j} e^{ikR_j} t_{0j}$

as

$$H = \sum_{k\sigma} \varepsilon_k c^{+}_{k\sigma} c_{k\sigma} + \frac{1}{N} \sum_{\substack{k,k',q,\\ \sigma,\sigma'}} V_{k,k',q} c^{+}_{k+q,\sigma} c^{+}_{k'-q,\sigma'} c_{k',\sigma'} c_{k,\sigma}$$

and find $V_{k,k',q}$ in terms of ε_k , α and U . Show all steps in your derivation.

Additional for 232 students:

Add to the Hamiltonian the term

$$H_V = \frac{1}{2} \sum_{i,j} V_{ij} n_i n_j$$

with $n_i = \sum_{\sigma} c^{+}_{i\sigma} c_{i\sigma}$ and find its contribution to $V_{k,k',q}$