Statistical Physics & Condensed Matter Theory I: Exercise

Superexchange and antiferromagnetism

We have seen in class that experimentally, the low-T Mott insulator is usually accompanied by **antiferromagnetic ordering** of local moments, and that this can be understood from the Hubbard model. This exercise aims at making this connection explicit.

Namely, we start with the Hubbard model,

$$\hat{H} = -t \sum_{\langle ij \rangle} a_{i\sigma}^\dagger a_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow},$$

where $a_{i\sigma}, a_{i\sigma}^\dagger$ are standard fermionic annihilation and creation operators (i labels sites, $\sigma = \uparrow, \downarrow$) for the vacuum $|0\rangle$, with anticommutation relations $\{a_{i\sigma}, a_{j\sigma'}^\dagger\} = \delta_{ij}\delta_{\sigma\sigma'}$, and $\hat{n}_{i\sigma} \equiv a_{i\sigma}^\dagger a_{i\sigma}$ are the number operators. More specifically, we will be interested in the strongly interacting limit $U/t \gg 1$ of the half-filled system (number of electrons = number of sites, so one electron per site on average).

We consider for simplicity the 'two-site' system. Writing the Hamiltonian as $\hat{H} = \hat{H}_t + \hat{H}_U$ we thus have for two sites $\hat{H}_t = -t \sum_\sigma (a_{1\sigma}^\dagger a_{2\sigma} + a_{2\sigma}^\dagger a_{1\sigma})$ and $\hat{H}_U = U \sum_{i=1,2} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$. At half filling, there are six possible states: two spin-polarized states, $a_{1\uparrow}^\dagger a_{2\uparrow}^\dagger |0\rangle$, $a_{1\downarrow}^\dagger a_{2\downarrow}^\dagger |0\rangle$, and four $S_{\text{tot}}^z = 0$ states, $|s_1\rangle \equiv a_{1\uparrow}^\dagger a_{2\downarrow}^\dagger |0\rangle$, $|s_2\rangle \equiv a_{2\uparrow}^\dagger a_{1\downarrow}^\dagger |0\rangle$, $|d_1\rangle \equiv a_{1\uparrow}^\dagger a_{1\downarrow}^\dagger |0\rangle$, $|d_2\rangle \equiv a_{2\uparrow}^\dagger a_{2\downarrow}^\dagger |0\rangle$.

The two spin-polarized states are already eigenstates, with zero energy. The four remaining eigenstates each involve superpositions of $|s_i\rangle$ and $|d_i\rangle$ representing singly- or doubly-occupied sites respectively. In the strong coupling limit $U/t \gg 1$, the ground state will consist predominantly of singly-occupied states $|s_i\rangle$, since the cost of double occupancy then completely overwhelms the kinetic part of the Hamiltonian. However, virtual hopping can still occur. This exercise aims at quantifying how this affects the physics.

a) Explicitly write down the action of $\hat{H}_t$ and $\hat{H}_U$ on the four $S_{\text{tot}}^z = 0$ states (express your answer in terms of linear combinations of those four states). Show that the Hamiltonian can thus be written as the following 4×4 matrix

$$\hat{H} = \begin{pmatrix} 0 & 0 & -t & -t \\ 0 & 0 & -t & -t \\ -t & -t & U & 0 \\ -t & -t & 0 & U \end{pmatrix} \equiv -t \begin{pmatrix} \mathbf{0} & \mathbf{f} \\ \mathbf{f} & \mathbf{0} \end{pmatrix} + U \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{pmatrix} = -t\sigma^x \otimes (\mathbf{1} + \sigma^x) + \frac{U}{2}(\mathbf{1} - \sigma^z) \otimes \mathbf{1}$$

when acting on vectors $(|s_1\rangle, |s_2\rangle, |d_1\rangle, |d_2\rangle)$. *In the second equality, we have conveniently written the 4×4 matrices as 2×2 matrices of 2×2 matrices, and then in the third equality as explicit tensor products, where $\mathbf{0}$ and $\mathbf{1}$ are respectively the 2×2 zero and unit matrices, and* $\mathbf{f} \equiv \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \mathbf{1} + \sigma^x$.

b) As we have seen in class, it is very natural to expect an effective Hamiltonian with residual interaction of order t^2/U in the strong coupling limit. We achieve this canonically, by looking for a transformation of the Hamiltonian in the S^z_{tot} subspace which cancels the order t operator part. A general canonical transformation can be parametrized as

$$\hat{H} \to \hat{H}' \equiv e^{it\hat{O}} \hat{H} e^{-it\hat{O}}$$

where $\hat{O}$ is the Hermitian operator effectuating the canonical transformation, and where we here insert t explicitly for convenience. Show that up to order t^2 (assuming $\hat{O}$ independent of t), we can write

$$\hat{H}' = \hat{H} + it[\hat{O}, \hat{H}] - \frac{t^2}{2!}[\hat{O}, [\hat{O}, \hat{H}]] + ...$$

and that the condition for vanishing of the linear order in t in $\hat{H}'$ is thus $\hat{H}_t + it[\hat{O}, \hat{H}_U] = 0$. Show that, provided we can find such an $\hat{O}$, we then get

$$\hat{H}' = \hat{H}_U + \frac{it}{2}[\hat{O}, \hat{H}_t] + O(t^3).$$

c) The crux of the problem is to find an operator $\hat{O}$ which does the order t cancellation. You can do this sub-question in **either** of the two following ways, using respectively matrix or operator algebra (the second way is like in the book).

i) **First way**: looking at the matrix for $\hat{H}$ (see a) above), brushing your teeth and using your intuition from Pauli matrices suggests that a form

$$\hat{O} = i\alpha \begin{pmatrix} \mathbf{0} & -\mathbf{f} \\ \mathbf{f} & \mathbf{0} \end{pmatrix} = \alpha\sigma^y \otimes \mathbf{f}$$

for the canonical transformation operator might do the trick. Show that it *does* work, provided α is chosen as $1/U$. *Hint: remember the mixed-product property of tensor products:* $(A \otimes B) \times (C \otimes D) = (A \times C) \otimes (B \times D)$ *where* $\times$ *is the normal matrix product.*

ii) **Second way**: define projection operators $\hat{P}_s$ and $\hat{P}_d$ onto respectively singly- and doubly-occupied subspaces,

$$\hat{P}_s = \sum_{i=1,2} |s_i\rangle\langle s_i|, \qquad \hat{P}_d = \sum_{i=1,2} |d_i\rangle\langle d_i|,$$

with $\hat{P}_s + \hat{P}_d = \mathbf{1}$. First, prove the following identities:

$$\hat{H}_U \hat{P}_s = 0 = \hat{P}_s \hat{H}_U, \qquad \hat{H}_U \hat{P}_d = U\hat{P}_d = \hat{P}_d \hat{H}_U, \qquad \hat{P}_s \hat{H}_t \hat{P}_s = 0 = \hat{P}_d \hat{H}_t \hat{P}_d.$$

Show, using these operator identities, that $\hat{O} = \frac{i}{Ut}[\hat{P}_s \hat{H}_t \hat{P}_d - \hat{P}_d \hat{H}_t \hat{P}_s]$ assures cancellation to first order in t, *i.e.* that $\hat{H}_t + it[\hat{O}, \hat{H}_U] = 0$.

N.B.: these two ways are of course the same, differing only in notation. The link is made by realizing that $P_s = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$ *and* $P_d = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{pmatrix}$ *and verifying that the two definitions of* $\hat{O}$ *are one and the same.*

d) Show that the canonically transformed Hamiltonian, projected onto the singly-occupied subspace, is

$$\hat{P}_s \hat{H}' \hat{P}_s = -2\frac{t^2}{U}(\sum_i |s_i\rangle\langle s_i| + |s_1\rangle\langle s_2| + |s_2\rangle\langle s_1|)$$

or, in matrix notation (for vectors $(|s_1\rangle, |s_2\rangle)$), $\hat{P}_s \hat{H}' \hat{P}_s = -2\frac{t^2}{U} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$.

e) The spin permutation operator $\mathbb{P}$ switches by definition spins on sites 1 and 2, *i.e.* $\mathbb{P}|s_1\rangle = \mathbb{P}a^\dagger_{1\uparrow}a^\dagger_{2\downarrow}|0\rangle = a^\dagger_{1\downarrow}a^\dagger_{2\uparrow}|0\rangle = -a^\dagger_{2\uparrow}a^\dagger_{1\downarrow}|0\rangle = -|s_2\rangle$ so this operator is represented in this subspace as $\mathbb{P} = -(|s_1\rangle\langle s_2| + |s_2\rangle\langle s_1|)$. Using our earlier result (seen in class) that the spin operators obey

$$\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 = -\frac{1}{4}\mathbf{1} + \frac{1}{2}\mathbb{P},$$

show that the resulting Hamiltonian becomes the famous **Heisenberg model**

$$P_s \hat{H}' P_s = J\left(\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 - \frac{1}{4}\right),$$

and give the value of J, which is the **antiferromagnetic exchange** strength.

The physical interpretation of this result is that neighbouring electrons with anti-parallel spins can take advantage of hybridization and reduce their kinetic energy by hopping. The Pauli principle prevents electrons with parallel spins from doing this. In the $U/t \gg 1$ limit, the charge modes do not have dynamics anymore: charges 'freeze', with one electron per site, and the system becomes an insulator (this is called the Mott-Hubbard transition). The spin dynamics however remains active, and antiferromagnetic in nature. This effective interaction, formulated by Anderson from ideas of Kramers, is known as **superexchange***, and is the most common source of antiferromagnetism in condensed matter.*