PHYS 6106, Graduate Quantum Mechanics II
Superexchange

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April 5, 2023

Contents

1 Introduction

This set of lecture notes is designed to introduce to concept of *magnetic superexchange* to graduate level physics students in an introductory quantum mechanics class. The topic is intended to demonstrate the utility of perturbation theory in deriving an effective Hamiltonian.

We will begin with a brief review of fermionic field operators. Next, we introduce the Hubbard Hamiltonian which serves as a toy model in condensed matter physics to describe Mott insulators. With this model, we perform the so called strong coupling expansion. Taking the deep Mott limit, we treat fermionic hopping as a perturbation. At half-filling, we show that the lowest nonvanishing perturbative correction to the Hamiltonian occurs at second order. Finally, we show that this second order correction is the antiferromagnetic Heisenberg Hamiltonian.

By the end of this lecture students should be able to

- follow algebraic manipulations of fermionic operators
- understand physical processes denoted by second quantized operators
- appreciate the utility of perturbation theory beyond energy corrections

2 Elements of Second Quantization

For normalized fermionic states in the position basis, $f_i(\mathbf{r})$, we may construct a fully antisymmetrized wavefunction by use of the Slater determinant

$$\Psi_{SD}(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} f_1(\mathbf{r}_1) & f_2(\mathbf{r}_1) & \cdots & f_N(\mathbf{r}_1) \\ f_1(\mathbf{r}_2) & f_2(\mathbf{r}_2) & \cdots & f_N(\mathbf{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ f_1(\mathbf{r}_N) & f_2(\mathbf{r}_N) & \cdots & f_N(\mathbf{r}_N) \end{vmatrix} \tag{1}$$

In second quantization, however, we work in the particle number occupation basis. We label many-particle Fock states by the number of fermions that occupy single-particle states. The vacuum state $|\Omega\rangle$ is the unique state with zero particles.

Fermionic creation and annihilation operators act on Fock states and increase or decrease the particle number respectively.

Letting i, j denote an arbitrary but unique labeling of quantum numbers, **fermionic field operators** are defined by the following algebra

$$\{c_i, c_j^\dagger\} = c_i c_j^\dagger + c_j^\dagger c_i = \delta_{ij} \tag{2}$$

and all other anticommutators zero.

From this we immediately have $c_i^2 = 0$ and $(c_i^\dagger)^2 = 0$. The vacuum state $|\Omega\rangle$ may be defined as the unique state such that $c_i |\Omega\rangle = 0$ for all i.

Second quantization of single particle operators: Single particle operators may be second quantized using their matrix representation. Given a matrix representation M_{ij} of a single particle operator, it is second quantized via

$$M = \sum_{ij} c_i^\dagger M_{ij} c_j \tag{3}$$

A review of second quantization may be found in [3].

3 Hubbard Hamiltonian

As a toy model to study insulators in condensed matter physics, we may use the second quantization formalism to write down a Hamiltonian consistent with the energetics we expect for electrons. First, there must be an energetic cost for electrons (with opposite spin projection) to be on the same lattice site. Generically, there is Coulombic repulsion further away from on site, but this repulsion dies off exponentially in the distance separating lattice sites [1]. We may further include a term that allows electrons to hop between lattice sites by annihilating them on-site, and creating them on a neighboring site. In doing so we obtain the Hubbard Hamiltonian.

The **Hubbard Hamiltonian** is given by

$$H = H_U + H_t = U \sum_i n_{i\uparrow} n_{i\downarrow} - t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + h.c.$$

where $U, t > 0$, $\sigma \in \{\uparrow, \downarrow\}$, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, and $\{c_{i\sigma}, c_{j\sigma'}^\dagger\} = \delta_{ij}\delta_{\sigma\sigma'}$.

H is the Hamiltonian, and it tells us the total energy of the system. The potential energy is given by H_U. The term H_U says there is an energetic cost, $U > 0$, when there are two fermions on the same lattice

site, i. This is a simple way to capture Coulombic repulsion between electrons on a lattice. When $t = 0$, the ground state energy of $H = H_U$ is minimized when all lattice sites are either unoccupied or singly occupied by a fermion.

The term H_t is the kinetic energy. This term says that the energy of the system is lowered by an amount, t, when a fermion "hops" from one lattice site to its nearest neighbor. Hopping does not affect the spin of the electron. By convention we take the kinetic term to lower the total energy of the system, although generically we may have $t \in \mathbb{C}$. Complex hopping t is outside the scope of these notes. For the purposes of superexchange, we take $t \in \mathbb{R}$.

4 Perturbation Theory and Effective Hamiltonians

In this section, we will use perturbation theory to derive an effective Hamiltonian for H under some reasonable constraints. First, we take a system with N sites and $U \gg t$ so that H_t is a perturbation. Moreover we will work at half filling so that there is one electron per lattice site.

The unperturbed Hamiltonian $H_0 = H_U$. The ground state manifold has a spin degeneracy and spans a Hilbert space of half-filled states denoted by $\mathbb{H}_0$. States in $\mathbb{H}_0$ are denoted by $|\phi\rangle \in \mathbb{H}_0$. Explicitly, $\sum_{\sigma\in\{\uparrow,\downarrow\}} n_{i\sigma} |\phi\rangle = |\phi\rangle$ for all $|\phi\rangle \in \mathbb{H}_0$.

The full Hamiltonian $H = H_U + H_t$, however, spans a larger Hilbert space $\mathbb{H}$. To compute the effective Hamiltonian H_{eff}, we will compute its matrix elements in the Hilbert space restricted to states at half-filling. That is $\langle\phi|H_{\text{eff}}|\phi'\rangle$ for all $|\phi\rangle, |\phi'\rangle \in \mathbb{H}_0$. These matrix elements may be computed using standard perturbation theory [2].

To second order in perturbation theory, the **effective Hamiltonian** is given by

$$\langle\phi|H_{\text{eff}}|\phi'\rangle = \langle\phi|H_U|\phi'\rangle + \langle\phi|H_t|\phi'\rangle + \sum_{k\notin\mathbb{H}_0} \frac{\langle\phi|H_t|k\rangle \langle k|H_t|\phi'\rangle}{E_0 - E_k} \tag{4}$$

We will first show that the zero and first order contributions vanish.

4.1 Zero Order Contribution

Since $|\phi\rangle, |\phi'\rangle \in \mathbb{H}_0$, they are at half-filling. Hence the total number of fermions on any $|\phi\rangle$ is always 1. Algebraically, $(n_{i\uparrow} + n_{i\downarrow}) |\phi\rangle = |\phi\rangle$ for all i. Rearranging, we have $n_{i\downarrow} |\phi\rangle = (1 - n_{i\uparrow}) |\phi\rangle$. Thus

$$\langle\phi|H_U|\phi'\rangle = U \sum_i \langle\phi|n_{i\uparrow}n_{i\downarrow}|\phi'\rangle = U \sum_i \langle\phi|n_{i\uparrow}(1 - n_{i\uparrow})|\phi'\rangle = 0 \tag{5}$$

Since $n_{i\uparrow}(1 - n_{i\uparrow}) = n_{i\uparrow} - n_{i\uparrow}^2 = n_{i\uparrow} - n_{i\uparrow} = 0$. The last equality follows since

$$n_{i\uparrow}^2 = c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\uparrow}^\dagger c_{i\uparrow} = c_{i\uparrow}^\dagger (1 - c_{i\uparrow}^\dagger c_{i\uparrow}) c_{i\uparrow} = c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\uparrow}^\dagger c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\uparrow} = n_{i\uparrow} - (c_{i\uparrow}^\dagger)^2 (c_{i\uparrow})^2 = n_{i\uparrow} \tag{6}$$

4.2 First Order Contribution

The first order contribution also vanishes. We note that $\mathbb{H}_0$ is not closed under the action of H_t. Physically, the action of terms in H_t on any state $|\phi'\rangle \in \mathbb{H}_0$ moves fermions from a given site i to a nearest neighbor site j. Since $|\phi'\rangle$ is at half-filling, however, site j has 1 fermion. Moving a fermion from site i to site j creates a doubly occupied site. Hence $H_t |\phi'\rangle \notin \mathbb{H}_0$ for any $|\phi'\rangle \in \mathbb{H}_0$. Explicitly, $H_t |\phi'\rangle \in \mathbb{H} \setminus \mathbb{H}_0$.

Since $\mathbb{H}$ is a Hilbert space, basis states in $\mathbb{H}$ are pairwise orthonormal. Therefore, if $H_t |\phi'\rangle \notin \mathbb{H}_0$ and $|\phi\rangle \in \mathbb{H}_0$, we must have $\langle\phi|H_t|\phi'\rangle = 0$. This is because states in $\mathbb{H}_0$ are orthogonal to states outside of $\mathbb{H}_0$.

4.3 Second Order Contribution

4.3.1 Single Particle Excitations

In this section we will show that the second order contribution is non-vanishing and given by

$$\sum_{k\notin\mathbb{H}_0}\frac{\langle\phi|H_t|k\rangle\langle k|H_t|\phi'\rangle}{E_0-E_k}=-\langle\phi|H_t\frac{\sum_j n_{j\uparrow}n_{j\downarrow}}{U}H_t|\phi'\rangle \tag{7}$$

Inspecting the right-hand side, we may insert a resolution of the identity as follows

$$-H_t\frac{\sum_j n_{j\uparrow}n_{j\downarrow}}{U}H_t=-H_t\sum_{k\in\mathbb{H}}\frac{\sum_j n_{j\uparrow}n_{j\downarrow}|k\rangle\langle k|}{U}H_t \tag{8}$$

Where we sum over the full Hilbert space $\mathbb{H}$. Let us inspect the term $n_{j\uparrow}n_{j\downarrow}|k\rangle$. We find

$$n_{j\uparrow}n_{j\downarrow}|k\rangle=\begin{cases}0, & |k\rangle\in\mathbb{H}_0\\ |k\rangle, & |k\rangle\notin\mathbb{H}_0,\quad\text{one doubly occupied site}\end{cases} \tag{9}$$

For half-filled states, $|k\rangle\in\mathbb{H}_0$, we may use an argument similar to that in 4.1 to show the above result. For $|k\rangle\notin\mathbb{H}_0$ and with one doubly occupied site, we obtain the above result. Formally, we may ignore states with more than one doubly occupied site. *This is because matrix elements of the form* $\langle\phi|H_t|k\rangle\langle k|H_t|\phi'\rangle$ *with* $|\phi\rangle,|\phi'\rangle\in\mathbb{H}_0$ *physically represent virtual tunning from the ground state manifold (half-filling) to itself via an excited state* $|k\rangle$ *with only one doubly occupied state.*

To see this, first examine $\langle k|H_t|\phi'\rangle$. The state $|\phi'\rangle$ is at half-filling, and the action of H_t creates all particle-hole excitations which create one vacant site and one doubly-occupied site next to the vacancy. For this matrix element not to vanish, $|k\rangle$ must be one of these states. A similar argument holds for $\langle\phi|H_t|k\rangle$. Crucially, however, the state $|k\rangle$ is the same for both matrix elements. Hence for the contribution to be non-vanishing, $|k\rangle$ must be a particle-hole excitation that connects $|\phi\rangle,|\phi'\rangle$ via a single hopping term. By restricting ourselves to matrix elements in $\mathbb{H}_0$, we need only consider the lowest lying excitations of the full Hilbert space $\mathbb{H}$.

With this in mind, we find

$$-\langle\phi|H_t\frac{\sum_j n_{j\uparrow}n_{j\downarrow}}{U}H_t|\phi\rangle=-\langle\phi|H_t\sum_{k\notin\mathbb{H}_0}\frac{|k\rangle\langle k|}{U}H_t|\phi\rangle \tag{10}$$

States with one doubly occupied site have energy

$$E_k=\langle k|H_0|k\rangle=U\sum_j\langle k|n_{j\uparrow}n_{j\downarrow}|k\rangle=U\sum_j\delta_{kj}\langle k|k\rangle=U \tag{11}$$

since the density-density term is only 1 on the doubly occupied site (i.e. where $k=j$ if we label the singly occupied site as k). The ground state manifold states have energy 0 since they have no doubly occupied states. Thus $-U=E_0-E_k$ and we have the desired result

$$-\langle\phi|H_t\frac{\sum_j n_{j\uparrow}n_{j\downarrow}}{U}H_t|\phi\rangle=\sum_{k\notin\mathbb{H}_0}\frac{\langle\phi|H_t|k\rangle\langle k|H_t|\phi'\rangle}{E_0-E_k} \tag{12}$$

4.3.2 Second Quantized form of Effective Hamiltonian

In the previous section we found the lowest order non-vanishing contribution to the effective Hamiltonian. Here, we will write this contribution in terms of fermionic operators and show it is given by

$$H_{\text{eff}}=-H_t\frac{\sum_j n_{j\uparrow}n_{j\downarrow}}{U}H_t=\frac{2t^2}{U}\sum_{\langle ij\rangle\sigma}\left(-n_{i\uparrow}n_{j\downarrow}+c^\dagger_{i\downarrow}c_{i\uparrow}c^\dagger_{j\uparrow}c_{j\downarrow}\right) \tag{13}$$

Physically, the first term says it is energetically favorable for nearest neighbor spins to point in opposite directions; the energy is lowered when nearest neighbor spins are anti-aligned. The second term says there is an energetic cost to flip a spin on a given site along with all of its neighbors.

Let us inspect the term $\sum_j n_{j\uparrow} n_{j\downarrow}$ in the above sum. This term will give nonzero matrix elements when there is at least one doubly occupied site. We can ensure this doubly occupied site exists, by sandwiching[1] the density-density term between $c^\dagger_{i\sigma} c_{j\sigma}$ on the left and $c^\dagger_{j\sigma'} c_{i\sigma'}$ on the right, with i, j nearest neighbors. Then

$$H_{\text{eff}} = -\frac{t^2}{U} \sum_{\langle ij \rangle \sigma\sigma'} c^\dagger_{i\sigma} c_{j\sigma} (n_{j\uparrow} n_{j\downarrow}) c^\dagger_{j\sigma'} c_{i\sigma'} \tag{14}$$

$$= -\frac{t^2}{U} \sum_{\langle ij \rangle \sigma\sigma'} c^\dagger_{i\sigma} c_{j\sigma} (c^\dagger_{j\uparrow} c_{j\uparrow} c^\dagger_{j\downarrow} c_{j\downarrow}) c^\dagger_{j\sigma'} c_{i\sigma'} \tag{15}$$

$$= \frac{t^2}{U} \sum_{\langle ij \rangle \sigma\sigma'} c^\dagger_{i\sigma} c_{j\sigma} (c^\dagger_{j\uparrow} c^\dagger_{j\downarrow} c_{j\uparrow} c_{j\downarrow}) c^\dagger_{j\sigma'} c_{i\sigma'} \tag{16}$$

where in the last line we have performed one anti-commutation to normal order the density-density term. Operator multiplication is associative, so we reorder the parentheses above.

$$H_{\text{eff}} = \frac{t^2}{U} \sum_{\langle ij \rangle \sigma\sigma'} (c^\dagger_{i\sigma} c_{j\sigma} c^\dagger_{j\uparrow} c^\dagger_{j\downarrow}) (c_{j\uparrow} c_{j\downarrow} c^\dagger_{j\sigma'} c_{i\sigma'}) \tag{17}$$

We may normal order each bracketed term to find

$$c^\dagger_{i\sigma} c_{j\sigma} c^\dagger_{j\uparrow} c^\dagger_{j\downarrow} = c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} - c^\dagger_{i\downarrow} c^\dagger_{j\uparrow}, \qquad c_{j\uparrow} c_{j\downarrow} c^\dagger_{j\sigma'} c_{i\sigma'} = c_{j\uparrow} c_{i\downarrow} - c_{j\downarrow} c_{i\uparrow} \tag{18}$$

where we have dropped quartic terms since $\mathbb{H}_0$ is not closed under their action (i.e. they do not contribute to the matrix element). The effective Hamiltonian then reads

$$H_{\text{eff}} = \frac{t^2}{U} \sum_{\langle ij \rangle \sigma} (c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} - c^\dagger_{i\downarrow} c^\dagger_{j\uparrow}) (c_{j\uparrow} c_{i\downarrow} - c_{j\downarrow} c_{i\uparrow}) \tag{19}$$

$$= \frac{t^2}{U} \sum_{\langle ij \rangle \sigma} c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} c_{j\uparrow} c_{i\downarrow} - c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} c_{j\downarrow} c_{i\uparrow} - c^\dagger_{i\downarrow} c^\dagger_{j\uparrow} c_{j\uparrow} c_{i\downarrow} + c^\dagger_{i\downarrow} c^\dagger_{j\uparrow} c_{j\downarrow} c_{i\uparrow} \tag{20}$$

$$= \frac{t^2}{U} \left\{ \sum_{\langle ij \rangle \sigma} -c^\dagger_{i\downarrow} c^\dagger_{j\uparrow} c_{j\uparrow} c_{i\downarrow} + c^\dagger_{i\downarrow} c^\dagger_{j\uparrow} c_{j\downarrow} c_{i\uparrow} + \sum_{\langle ij \rangle \sigma} -c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} c_{j\downarrow} c_{i\uparrow} + c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} c_{j\uparrow} c_{i\downarrow} \right\} \tag{21}$$

In the last line we have simply reordered the sum and broken it up via linearity. Note that the second sum is equivalent to the first by interchanging $i \to j$. Thus

$$H_{\text{eff}} = \frac{2t^2}{U} \sum_{\langle ij \rangle \sigma} -c^\dagger_{i\downarrow} c^\dagger_{j\uparrow} c_{j\uparrow} c_{i\downarrow} + c^\dagger_{i\downarrow} c^\dagger_{j\uparrow} c_{j\downarrow} c_{i\uparrow} \tag{22}$$

$$= \frac{2t^2}{U} \sum_{\langle ij \rangle \sigma} -c^\dagger_{i\downarrow} c_{i\downarrow} c^\dagger_{j\uparrow} c_{j\uparrow} + c^\dagger_{i\downarrow} c_{i\uparrow} c^\dagger_{j\uparrow} c_{j\downarrow} \tag{23}$$

$$= \frac{2t^2}{U} \sum_{\langle ij \rangle \sigma} -n_{i\uparrow} n_{j\uparrow} + c^\dagger_{i\downarrow} c_{i\uparrow} c^\dagger_{j\uparrow} c_{j\downarrow} \tag{24}$$

where in the penultimate line we have performed two anti-commutations.

[1] Formally these operators come from H_t. Expanding out H_t performing some algebraic manipulations gives us the same result, but our physical intuition here for doubly occupied sites saves us from some calculations.

To second order in perturbation theory, the effective Hamiltonian reads

$$H_{\text{eff}} = \frac{2t^2}{U} \sum_{\langle ij \rangle \sigma} -n_{i\uparrow} n_{j\uparrow} + c^\dagger_{i\downarrow} c_{i\uparrow} c^\dagger_{j\uparrow} c_{j\downarrow} \tag{25}$$

5 Heisenberg Hamiltonian

With very little physical motivation, we now second quantize spin operators on each site. While this step is not well motivated a priori, applying it to our problem will provide us with some well needed physical intuition.

Using (3), we second quantize the spin operators ($\hbar = 1$) as follows

$$S^z_i = \sum_{\sigma\sigma'} c^\dagger_{i\sigma} \left(\frac{1}{2} \sigma^z_{\sigma\sigma'} \right) c_{i\sigma'} = \frac{1}{2}(c^\dagger_{i\uparrow} c_{i\uparrow} - c^\dagger_{i\downarrow} c_{i\downarrow}) = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow}) \tag{26}$$

$$S^+_i = \sum_{\sigma\sigma'} c^\dagger_{i\sigma} \left(\sigma^+_{\sigma\sigma'} \right) c_{i\sigma'} = c^\dagger_{i\uparrow} c_{i\downarrow} \tag{27}$$

$$S^-_i = \sum_{\sigma\sigma'} c^\dagger_{i\sigma} \left(\sigma^-_{\sigma\sigma'} \right) c_{i\sigma'} = c^\dagger_{i\downarrow} c_{i\uparrow} \tag{28}$$

Physically, S^z_i represents the local magnetization on site i. We may compute this by counting the number of spin up fermions on the site and subtracting the number of spin down fermions on the same site. The spin raising and lowering operators amount to flipping the spin of a fermion on a given site, and we represent this as an on-site hopping term as above.

Returning to the effective Hamiltonian, we may summing over σ, perform an index change $i \to j$, and perform some anticommutations allows us to rewrite it as

$$H_{\text{eff}} = \frac{2t^2}{U} \sum_{\langle ij \rangle} -(n_{i\uparrow} n_{j\uparrow} + n_{i\downarrow} n_{j\uparrow}) + c^\dagger_{i\downarrow} c_{i\uparrow} c^\dagger_{j\uparrow} c_{j\downarrow} + c^\dagger_{i\uparrow} c_{i\downarrow} c^\dagger_{j\downarrow} c_{j\uparrow} \tag{29}$$

We recognize the positive quartic terms as $S^+_i S^-_j + h.c.$ so that

$$H_{\text{eff}} = \frac{2t^2}{U} \sum_{\langle ij \rangle} -(n_{i\uparrow} n_{j\uparrow} + n_{i\downarrow} n_{j\uparrow}) + (S^+_i S^-_j + h.c.) \tag{30}$$

This motivates studying the density-density terms may as related to $S^z_i S^z_j$.

$$2S^z_i S^z_j = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})(n_{j\uparrow} - n_{j\downarrow}) = \frac{1}{2}(n_{i\uparrow} n_{j\uparrow} + n_{i\downarrow} n_{j\downarrow} - n_{i\uparrow} n_{j\downarrow} - n_{i\downarrow} n_{j\uparrow}) \tag{31}$$

Within $\mathbb{H}_0$, $n_{i\uparrow} + n_{i\downarrow} = 1$ (half-filling). Using this constraint on i, j,

$$2S^z_i S^z_j = \frac{1}{2}((1 - n_{i\downarrow}) n_{j\uparrow} + (1 - n_{i\uparrow}) n_{j\downarrow} - n_{i\downarrow} n_{j\uparrow} - n_{i\uparrow} n_{j\downarrow}) \tag{32}$$

$$= \frac{1}{2}((n_{j\uparrow} + n_{j\downarrow}) - 2n_{i\downarrow} n_{j\uparrow} - 2n_{i\uparrow} n_{j\downarrow}) \tag{33}$$

$$= 1 - n_{i\downarrow} n_{j\uparrow} - n_{i\uparrow} n_{j\downarrow} \tag{34}$$

The quartic terms are the density-density terms in the effective Hamiltonian. Hence we have

$$H_{\text{eff}} = \frac{2t^2}{U} \sum_{\langle ij \rangle} 2S^z_i S^z_j + (S^+_i S^-_j + h.c.) - \frac{1}{2} \tag{35}$$

We find that the low-energy effective theory of a Hubbard Hamiltonian at half-filling in the strong coupling limit ($U \gg t$) is the **antiferromagnetic Heisenberg model**:

$$H_{\text{eff}} = \frac{4t^2}{U} \sum_{\langle ij \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} \right) \tag{36}$$

At low energies, the predominant excitations of the Hubbard model at half-filling are antiferromagnetic. Classically, such a Hamiltonian causes spins on neighboring lattice sites to align in opposite directions. Quantum mechanical effects on this model have been extensively studied, but they are outside the scope of these notes.

References

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