Concepts in Condensed Matter Physics: Tutorial I

Tight Binding and The Hubbard Model

"Everything should be made as simple as possible, but no simpler"

– A. Einstein

1 Introduction

The Hubbard Hamiltonian (HH) offers one of the most simple ways to get insight into how the interactions between electrons give rise to insulating, magnetic, and even novel superconducting effects in a solid. It was written down [1, 2, 3, 4] in the early 1960's and initially applied to the behavior of the transition-metal monoxides (FeO, NiO, CoO), compounds which are antiferromagnetic insulators, yet had been predicted to be metallic by methods which treat strong interactions less carefully.

Over the intervening years, the HH has been applied to many systems, from "heavy fermions" and the Cerium volume collapse transition in the 1980's, to high temperature superconductors in the 1990's. Indeed, it is an amazing feature of the HH that, despite its simplicity, it exhibits behavior relevant to many of the most subtle and beautiful properties of solid state systems. We focus here for the most part on the single-band HH. Multi-band variants like the Periodic Anderson Model (PAM) allow one to introduce other fundamental concepts in many-body physics, such as the competition between magnetic order and singlet formation. Randomness can be simply introduced into the HH, so it can be used as a starting point for investigations of the interplay of interactions and disorder in metal-insulator transitions and, recently, many-body localization. "Textbook" discussions of the HH can be found in Refs. [5, 6, 7, 8] and a recent celebration of its 50th anniversary [9] emphasizes the resurgence of interest due to optical lattice emulation experiments.

2 Tight binding method

Consider a lattice of static Ions creating a periodic potential,

$$V_{\text{Lattice}}\left(\vec{r}\right) = \sum_{\vec{R}} V_{\text{Ion}}\left(\vec{r} - \vec{R}\right) = \sum_{\vec{R}} V_{\text{Ion}}^{\vec{R}}\left(\vec{r}\right) \ , \tag{1}$$

where $\vec{R}$ points to the lattice sites and $V_{\text{Ion}}^{\vec{R}}\left(\vec{r}\right) = V_{\text{Ion}}\left(\vec{r} - \vec{R}\right)$ is the potential of the Ion positioned at $\vec{R}$. In the limit of infinitely far away Ions we can solve the system by solving the Ions independently,

$$\left[\frac{\vec{p}^2}{2m} + V_{\text{Ion}}^{\vec{R}}\left(\vec{r}\right)\right] \phi_n^{\vec{R}}\left(\vec{r}\right) = \epsilon_n^{\vec{R}} \phi_n^{\vec{R}}\left(\vec{r}\right) \ , \tag{2}$$

where $\phi_n^{\vec{R}}\left(\vec{r}\right) = \phi_n\left(\vec{r} - \vec{R}\right)$ is the eigenstate of the nth orbital of the Ions positioned at $\vec{R}$, with corresponding energy $\epsilon_n^{\vec{R}}$. The total energy and wavefunction are:

$$E = \sum_{i=1}^{N} \epsilon_{n_i}^{\vec{R}_i} \ , \tag{3a}$$

$$\Phi = Slater\left[\left\{\phi_{n_i}^{\vec{R}_i}\right\}_{i=1}^{N}\right] \ , \tag{3b}$$

where N is the total number of electrons. Upon bringing the Ions closer together there are two main differences to consider:

1. Each site $\vec{R}$ start feeling the potential due to the other sites $\vec{R}'$. This leads to a small correction to the single Ion potential: $\Delta V_{\vec{R}}\left(\vec{r}\right) = \sum_{\vec{R}' \neq \vec{R}} V_{\text{Ion}}^{\vec{R}'}\left(\vec{r}\right)$.

2. The wavefunctions corresponding to different Ions, positioned at $\vec{R}$ and $\vec{R}'$, begin to overlap: $\langle \phi_m^{\vec{R}'} | \phi_n^{\vec{R}} \rangle \neq 0$.

Therefore, we do perturbation theory in $\Delta V_{\vec{R}}$, which to first order gives a matrix element for electron tunnelling between sites and orbitals,

$$t_{n,m}^{\vec{R},\vec{R}'} \equiv -\langle \phi_n^{\vec{R}} | \Delta V_{\vec{R}'} | \phi_m^{\vec{R}'} \rangle \ . \tag{4}$$

It should be noted that, as addressed in point number two above, the set of wavefunctions $| \phi_n^{\vec{R}} \rangle$ are not orthogonal and extra care should be taken to properly derive the tunneling

matrix element $t_{n,m}^{\vec{R},\vec{R}'}$. However, we will not dwell on this more in this course. The tight-binding method will be taught in a rigorous manner in the next course, Solid State 2, and can be found also in Ashcroft and Mermin's book [10]. We have so far disregarded the electron spin completely. Adding it is straightforward though, since the potential does not depend on it at all. The eigenstates will simply carry also a spin index, on which the energies are degenerate, and the hopping matrix element t will be diagonal in spin.

In 2$^{\text{nd}}$ quantization we define creation and annihilation operators,

$$c_{\vec{R},n,\sigma}^{\dagger} = \int d^3r \, \phi_{\vec{R},n,\sigma}(\vec{r}) \psi^{\dagger}(\vec{r}) \ , \tag{5a}$$

$$c_{\vec{R},n,\sigma} = \int d^3r \, \phi_{\vec{R},n,\sigma}^*(\vec{r}) \psi(\vec{r}) \ , \tag{5b}$$

satisfying $\left\{ c_{\vec{R},n,\sigma}, c_{\vec{R}',m,\sigma'}^{\dagger} \right\} = \delta_{\vec{R},\vec{R}'} \delta_{n,m} \delta_{\sigma,\sigma'}$, and the Hamiltonian takes the form

$$H = \sum_{\vec{R},n,\sigma} \epsilon_{\vec{R},n} c_{\vec{R},n,\sigma}^{\dagger} c_{\vec{R},n,\sigma} - \sum_{\vec{R},\vec{R}',n,m,\sigma} \left(t_{n,m}^{\vec{R},\vec{R}'} c_{\vec{R},n,\sigma}^{\dagger} c_{\vec{R}',m,\sigma} + h.c. \right) \ . \tag{6}$$

Before adding electron-electron interactions we will make some simplifications. Some are very widely used, and some are just for our own convenience:

1. We will consider only a single orbital per site, and drop the index n. This is not justified in all systems, but will be enough for our purposes.

2. Since the matrix element for electron hopping, $t_{\vec{R},\vec{R}'}$, decays exponentially with $\left| \vec{R} - \vec{R}' \right|$, we will truncate it after nearest neighbours (n.n.). Namely, $t_{\vec{R},\vec{R}'}$ does not vanish only for n.n. sites, denoted by $\langle \vec{R}, \vec{R}' \rangle$.

3. We will assume that all Ions are identical, and set $\epsilon_{\vec{R}} \equiv \mu$ for all $\vec{R}$ as well as $t_{\langle \vec{R}, \vec{R}' \rangle} \equiv t$ for all n.n. $\vec{R}$ and $\vec{R}'$. Systems where this assumption is wrong are called "inhomogeneous". In reality all systems are inhomogeneous, but usually the inhomogeneity is weak, and can be neglected or treated in perturbation theory.

Armed with these simplifications, and specializing to one dimension (1d), the system is described by the Hamiltonian,

$$H = \mu \sum_{j,\sigma} c_{j,\sigma}^{\dagger} c_{j,\sigma} - t \sum_{j,\sigma} \left(c_{j,\sigma}^{\dagger} c_{j+1,\sigma} + c_{j+1,\sigma}^{\dagger} c_{j,\sigma} \right) \ . \tag{7}$$

For the rest of the tutorial we will work at half filling, namely one electron per site. Notice that for a fixed number of electrons the μ term is just a constant, and so we will drop it.

To solve this Hamiltonian we use the (discrete) Fourier transform[1]

$$c_{k,\sigma} = \frac{1}{\sqrt{N}} \sum_j e^{-ikx_j} c_{j,\sigma} \ , \tag{8a}$$

$$c_{j,\sigma} = \frac{1}{\sqrt{N}} \sum_k e^{ikx_j} c_{k,\sigma} \ , \tag{8b}$$

where N is the number of sites and $k_n = \frac{2\pi n}{L}$, where $L = Na$ is the length of the system. Notice that $c_{k+\frac{2\pi}{a},\sigma} = c_{k,\sigma}$, so k-space is $\frac{2\pi}{a}$ periodic and it is enough to consider the region $k \in \left[-\frac{\pi}{a}, \frac{\pi}{a} \right)$, namely the first Brillouin Zone (BZ1). Plugging Eq.(8) into Eq.(7) (dropping the μ term) we diagonalize the Hamiltonian

$$
\begin{aligned}
H &= \sum_{k,q,\sigma} \left[-t c_{k,\sigma}^\dagger c_{q,\sigma} (e^{iq} + e^{-ik}) \right] \frac{1}{N} \sum_j e^{-i(k-q)x_j} \\
&= \sum_{k,q,\sigma} \left[-t c_{k,\sigma}^\dagger c_{q,\sigma} (e^{iqa} + e^{-ika}) \right] \delta_{k,q} \\
&= \sum_{k,\sigma} \left[-2t \cos(ka) \right] c_{k,\sigma}^\dagger c_{k,\sigma} \ ,
\end{aligned}
\tag{9}
$$

where we used the fact that $\frac{1}{N} \sum_j e^{-i(k-q)x_j} = \delta_{k,q}$. The solution is depicted in Fig.1. In order to count the number of states we notice that they are spaced $\Delta k = \frac{2\pi}{Na}$ apart spanning $k_{\max} - k_{\min} = \frac{2\pi}{a}$. The number of states is then given by,

$$2 \frac{k_{\max} - k_{\min}}{\Delta k} = 2N, \tag{10}$$

where the factor of 2 is for spin. At half filling (one electron per site, i.e., N electrons) the ground state has the lowest N states occupied. The system is therefore gapless, meaning that it can be excited above the ground state by any infinitesimal energy injection (or temperature). A gapless system of electron is called metallic, since it conducts.

In order to introduce a gap, consider a dimerization of the lattice such that all even sites

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[1]One can use various definitions for the Fourier transform, but the symmetric $\frac{1}{\sqrt{N}}$ convention ensures $c_{k,\sigma}^\dagger$ and $c_{k,\sigma}$ are indeed creation and annihilation operators, i.e., have appropriate anti-commutation relations $\left\{ c_{k,\sigma}, c_{q,\sigma'}^\dagger \right\} = \delta_{k,q} \delta_{\sigma,\sigma'}$.
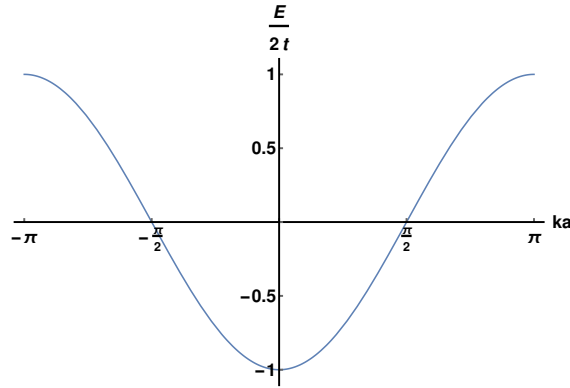
Figure 1: Spectrum of a free fermion on a 1d lattice in the tight-binding approximation. The energy band is doubly degenerate in the spin degree of freedom. At half filling all state below zero (between $-\pi/2$ and $\pi/2$) are filled.

are slightly displaced from their position[2]. Instead of changing the distance between Ions we will use a trick and change the tunneling matrix element,

$$t_{j,j+1} = t \left[1 + \Delta(-1)^j \right], \tag{11}$$

where Δ is governed by the displacement of the Ions. Indeed doing so captures essentially the same physics since, as can be seen in Eq.(4), the size of t relates to the distance between Ions. Notice that now the symmetry for translation by a is broken, and one must define a unit cell of size $2a$ with two Ions in the unit cell. We will denote the creation operators on odd sites by $A_{j,\sigma}^\dagger$ and those on even by $B_{j,\sigma}^\dagger$. The Hamiltonian can now be written as

$$H = -t(1-\Delta) \sum_{j,\sigma} \left(A_{j,\sigma}^\dagger B_{j,\sigma} + B_{j,\sigma}^\dagger A_{j,\sigma} \right) - t(1+\Delta) \sum_{j,\sigma} \left(A_{j+1,\sigma}^\dagger B_{j,\sigma} + B_{j,\sigma}^\dagger A_{j+1,\sigma} \right) . \tag{12}$$

We now transform again to k-space using the definitions (8), but with $2a$ and $\frac{N}{2}$ unit cells

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[2]In reality, such a dimerization is always energetically favorable in 1d system at half filling, since as the gap opens the (occupied) states near the middle of the gap lower their energy. This lower energy overcomes the energy cost of displacing the Ions. Therefore, the lattice will spontaneously break the translation symmetry from a to $2a$, leading to an insulator rather than a metal. This effect is called Peierls instability, or Peierls transition.

to get

$$H = \sum_{k,\sigma} \vec{C}_{k,\sigma}^{\dagger} \begin{pmatrix} 0 & -t' - \tilde{t}e^{i2ka} \\ -t' - \tilde{t}e^{-i2ka} & 0 \end{pmatrix} \vec{C}_{k,\sigma} \equiv \sum_{k,\sigma} \vec{C}_{k,\sigma}^{\dagger} H(k) \vec{C}_{k,\sigma} \ , \qquad (13)$$

where $\vec{C}_{k,\sigma} = \begin{pmatrix} A_{k,\sigma} & B_{k,\sigma} \end{pmatrix}^{T}$, $t' = t(1 - \Delta)$ and $\tilde{t} = t(1 + \Delta)$. To completely solve the system we just need to diagonalize withing the unit cell, namely the two-by-two matrix $H(k)$. This can be done easily by first noticing that

$$H(k) = \vec{d}_{k} \cdot \vec{\tau} = |d_{k}| \, \vec{n} \cdot \vec{\tau}, \qquad (14)$$

where $\vec{n} = \begin{pmatrix} \cos 2\theta_{k} & \sin 2\theta_{k} & 0 \end{pmatrix}$ is a unit vector, $\vec{\tau}$ is a vector of Pauli matrices (here not related to the spin degree of freedom but rather to "pseudo spin"), $|d_{k}|$ is the mudulus of $\vec{d}_{k}$ and $\theta_{k} = \frac{1}{2} \arctan \left[\frac{\tilde{t} \sin(2ka)}{-t' - \tilde{t} \cos(2ka)} \right]$. The energies and eigenstates are then

$$E_{\pm}(k) = \pm |d_{k}| = \pm 2t \sqrt{1 - (1 - \Delta^{2}) \sin^{2}(ka)} \ , \qquad (15a)$$

$$\Gamma_{\pm}(k) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i2\theta_{k}} \\ \pm 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \left(e^{-i2\theta_{k}} A_{k,\sigma} \pm B_{k,\sigma} \right) \ , \qquad (15b)$$

and are depicted in Fig.2 for $\Delta = 0.2$. Notice that there are two bands now, corresponding to the two sites in the unit cell, and a gap between them. At half filling the lower band is completely full, while the upper is completely empty, and the system is gapped. Meaning that exciting the system requires overcoming a finite energy gap, in this case 2Δ. For example, thermal excitation of the system is suppressed by a Boltzman factor of $\exp[-k_{B}T/2\Delta]$. A gapped system of electrons is called insulating since it does not conduct.

3 The Hubbard Model

After playing around with the simplest non-interacting tight binding model we are ready to add interactions. We will do so in three dimensions (3d). Consider electron-electron interactions of the form

$$V_{\text{el-el}} = \sum_{\sigma,\sigma'} \int d^{3}r d^{3}r' V(\vec{r} - \vec{r}') \psi_{\sigma}^{\dagger}(\vec{r}) \psi_{\sigma'}^{\dagger}(\vec{r}') \psi_{\sigma'}(\vec{r}') \psi_{\sigma}(\vec{r}) \ , \qquad (16)$$
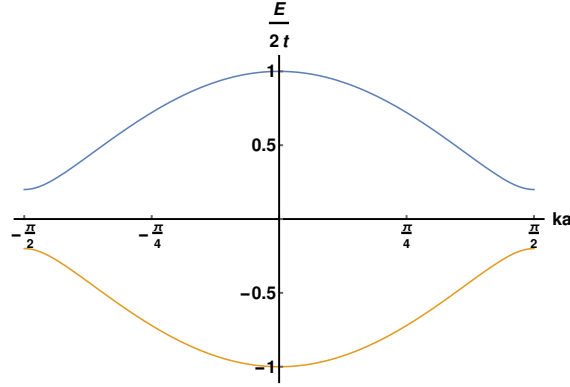
Figure 2: Spectrum of a free fermion on a dimerized 1d lattice in the tight-binding approximation. Both energy bands are doubly degenerate in the spin degree of freedom. At half filling the lower band is filled, while the upper is completely empty.

where $V(\vec{r} - \vec{r}')$ could for example be Coulomb repulsion. In the tight binding approximation, roughly speaking using Eq.(5), the interactions are given by

$$\tilde{V}_{\text{el–el}} = \sum_{\vec{R}} U_{\vec{R},\vec{R}} n_{\vec{R},\uparrow} n_{\vec{R},\downarrow} + \sum_{\vec{R}' \neq \vec{R}} U_{\vec{R},\vec{R}'} n_{\vec{R}} n_{\vec{R}'} + \sum_{\vec{R}' \neq \vec{R},\sigma,\sigma'} J^F_{\vec{R},\vec{R}'} c^\dagger_{\vec{R},\sigma} c^\dagger_{\vec{R}',\sigma'} c_{\vec{R},\sigma'} c_{\vec{R}',\sigma} \ , \tag{17}$$

where $n_{\vec{R}} = \sum_\sigma n_{\vec{R},\sigma}$ is the electron density on the site positioned at $\vec{R}$, $n_{\vec{R},\sigma}$ is the density of electrons of spin σ on the site positioned at $\vec{R}$, and the various matrix elements are:

$$U_{\vec{R},\vec{R}'} = \frac{1}{2} \int d^3 r_1 d^3 r_2 V(\vec{r}_1 - \vec{r}_2) \left| \phi_{\vec{R}}(\vec{r}_1) \right|^2 \left| \phi_{\vec{R}'}(\vec{r}_2) \right|^2 \ , \tag{18a}$$

$$J^F_{\vec{R},\vec{R}'} = \frac{1}{2} \int d^3 r_1 d^3 r_2 V(\vec{r}_1 - \vec{r}_2) \phi_{\vec{R}}(\vec{r}_1) \phi^*_{\vec{R}'}(\vec{r}_1) \phi_{\vec{R}'}(\vec{r}_2) \phi^*_{\vec{R}}(\vec{r}_2) \ . \tag{18b}$$

Notice that again we have three free parameters reminiscent of the "three channels". Here however, $J^F_{\vec{R},\vec{R}'}$ is very small compared to $U_{\vec{R},\vec{R}'}$, since it includes two overlap integrals of wavefunctions centered around different sites. By far the most important term in Eq.(17) is $U_{\vec{R},\vec{R}}$. Consequently, the other terms are commonly truncated[3] resulting in the so-called Hubbard model

$$H_{\text{Hubbard}} = -t \sum_{\langle \vec{R},\vec{R}' \rangle,\sigma} \left(c^\dagger_{\vec{R},\sigma} c_{\vec{R}',\sigma} + h.c. \right) + U \sum_{\vec{R}} n_{\vec{R},\uparrow} n_{\vec{R},\downarrow} \ , \tag{19}$$

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[3]We will return to the $J^F_{\vec{R},\vec{R}'}$ term later on in this tutorial.

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where $U = U_{\vec{R},\vec{R}}$ which again is assumed to be the same for all $\vec{R}$. Although we have omitted many terms that in reality are present, the resulting simplified model is still surprisingly rich. Moreover, even though it is arguably the simplest interacting electron model one can write down, we do not know how to solve it exactly. Therefore, we will consider various limits.

We already treated the $U = 0$ case in 1d. Generalizing it to 3d is straightforward, and we will skip it. One can treat $U \ll t$ using perturbation theory in $\frac{U}{t}$. It does not lead to dramatic effects, and we will skip that as well. Interesting results occur for the $t = 0$ and $t \ll U$ limits, and so we will focus on these. For $t = 0$ the Hamiltonian reduces to

$$H_0 = U \sum_{\vec{R}} n_{\vec{R},\uparrow} n_{\vec{R},\downarrow} \ , \tag{20}$$

for which the (degenerate) ground states can be easily inferred for any number of electrons. At half filling the ground state energy is $E = 0$ and the ground states have all sites occupied by a single electron. Lowest excited states, those that have one doubly occupied site, have a finite energy U, so the system is again gapped, but now due to interactions (rather than band-structure). This is called a Mott insulator. As opposed to a band insulator, which is completely inert, in this Mott insulator there are still low energy degrees of freedom, namely the spins of the electrons

$$S_{\vec{R}}^{\mu} = \frac{1}{2} \sum_{s,s'} c_{\vec{R},s}^{\dagger} \sigma_{s,s'}^{\mu} c_{\vec{R},s'} \ . \tag{21}$$

The many degenerate ground states correspond to all possible configurations of the spins of the electrons. This degeneracy is lifted by any finite t leading to a tunneling Hamiltonian,

$$H_t = -t \sum_{\langle \vec{R},\vec{R}' \rangle, \sigma} \left(c_{\vec{R},\sigma}^{\dagger} c_{\vec{R}',\sigma} + h.c. \right) \ , \tag{22}$$

which will prefer certain spin configurations. We will treat H_t in perturbation theory and derive an effective Hamiltonian for the degenerate ground space. To second order in perturbation theory the effective Hamiltonian is given by

$$H_{\text{eff}} = P_0 H_t P_0 + P_0 H_t P_1 \frac{1}{E_0 - H_0} P_1 H_t P_0 + O\left(\frac{t^3}{U^2} \right) \ , \tag{23}$$

where $P_0 = \sum_{\alpha \in \text{g.s.}} |\alpha\rangle \langle\alpha|$ is the projection operator to the ground space, and $P_1 = 1 - P_0 = \sum_{a \notin \text{g.s.}} |a\rangle \langle a|$ is the complementary projection. The first term in Eq.(23) clearly vanishes since H_t connects states in P_0 with states in P_1 which are the orthogonal to states

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in P_0. The second term can be simplified by noting:

1. The g.s. energy is zero, namely $E_0 = 0$.

2. Since H_t acting on states in P_0 creates only one double occupied site, all states in $P_1 H_t P_0$ have exactly one doubly occupied site.

We can then write:

$$
\begin{aligned}
H_{\text{eff}} &= \sum_{\alpha,\beta\in\text{g.s.}} \sum_{a,b\in 1 \text{ d.o.}} |\alpha\rangle \langle\alpha|H_t|a\rangle \langle a|\frac{1}{-H_0}|b\rangle \langle b|H_t|\beta\rangle \langle\beta| + O\left(\frac{t^3}{U^2}\right) \\
&= -\frac{1}{U} \sum_{\alpha,\beta\in\text{g.s.}} \sum_{a,b\in 1 \text{ d.o.}} |\alpha\rangle \langle\alpha|H_t|a\rangle \langle a|b\rangle \langle b|H_t|\beta\rangle \langle\beta| + O\left(\frac{t^3}{U^2}\right) \\
&= -\frac{1}{U} \sum_{\alpha,\beta\in\text{g.s.}} \sum_{a\in 1 \text{ d.o.}} |\alpha\rangle \langle\alpha|H_t|a\rangle \langle a|H_t|\beta\rangle \langle\beta| + O\left(\frac{t^3}{U^2}\right) \\
&= -\frac{1}{U} \sum_{\alpha,\beta\in\text{g.s.}} \langle\alpha|H_t^2|\beta\rangle |\alpha\rangle \langle\beta| + O\left(\frac{t^3}{U^2}\right) \;,
\end{aligned}
\tag{24}
$$

So we need to compute that Matrix elements $\langle\alpha|H_t^2|\beta\rangle$. Since $H_t = \sum_{\langle\vec{R},\vec{R}'\rangle}(H_t)_{\vec{R},\vec{R}'}$ only connect n.n. we concentrate on the spin configuration of two specific n.n. sites $\vec{R}$ and $\vec{R}'$. We denote the states in short $|\beta\rangle = |\cdots,\sigma_{\vec{R}},\sigma'_{\vec{R}'},\cdots\rangle \equiv |\sigma_{\vec{R}},\sigma'_{\vec{R}'}\rangle$, and look at the various cases:

(I) If both spins are oriented at the same direction, namely $|\beta\rangle = |\uparrow_{\vec{R}},\uparrow_{\vec{R}'}\rangle$ or $|\beta\rangle = |\downarrow_{\vec{R}},\downarrow_{\vec{R}'}\rangle$, they will be annihilated by $(H_t)_{\vec{R},\vec{R}'}$ since the site $\vec{R}$ (or $\vec{R}'$) cannot be occupied by two electrons with the same spin (Pauli exclusion principle):

$$
(H_t)_{\vec{R},\vec{R}'} |\sigma_{\vec{R}},\sigma_{\vec{R}'}\rangle = 0 \;.
\tag{25}
$$

(II) If the spins are opposite, namely $|\beta\rangle = |\uparrow_{\vec{R}},\downarrow_{\vec{R}'}\rangle$ or $|\beta\rangle = |\downarrow_{\vec{R}},\uparrow_{\vec{R}'}\rangle$, then $(H_t)_{\vec{R},\vec{R}'}$ leads to a doubly occupied site $\vec{R}$ or $\vec{R}'$:

$$
(H_t)_{\vec{R},\vec{R}'} |\sigma_{\vec{R}},\bar{\sigma}_{\vec{R}'}\rangle = -t|\sigma_{\vec{R}}\bar{\sigma}_{\vec{R}},0\rangle - t|0,\sigma_{\vec{R}'}\bar{\sigma}_{\vec{R}'}\rangle \;.
\tag{26}
$$

The second $(H_t)_{\vec{R},\vec{R}'}$ then splits them back onto both sites, by either going back to the original state or by exchanging the electrons:

(a) Back to original state:

$$(H_t)^2_{\vec{R},\vec{R}'} \, | \, \sigma_{\vec{R}}, \bar{\sigma}_{\vec{R}'} \, \rangle = 2t^2 \, | \, \sigma_{\vec{R}}, \bar{\sigma}_{\vec{R}'} \, \rangle \; . \tag{27}$$

(b) Exchanged electrons:

$$(H_t)^2_{\vec{R},\vec{R}'} \, | \, \sigma_{\vec{R}}, \bar{\sigma}_{\vec{R}'} \, \rangle = -2t^2 \, | \, \bar{\sigma}_{\vec{R}}, \sigma_{\vec{R}'} \, \rangle \; . \tag{28}$$

The extra minus sign in this case comes from the exchange of the electrons, and can be seen explicitly:

$$\begin{aligned}
(H_t)^2_{\vec{R},\vec{R}'} \, | \, \sigma_{\vec{R}}, \bar{\sigma}_{\vec{R}'} \, \rangle &= (H_t)_{\vec{R},\vec{R}'} \left(-t c^\dagger_{\vec{R}',\uparrow} c_{\vec{R},\uparrow} - t c^\dagger_{\vec{R},\downarrow} c_{\vec{R}',\downarrow} \right) | \, \sigma_{\vec{R}}, \bar{\sigma}_{\vec{R}'} \, \rangle \\
&= \left[\left(-t c^\dagger_{\vec{R},\downarrow} c_{\vec{R}',\downarrow} \right) \left(-t c^\dagger_{\vec{R}',\uparrow} c_{\vec{R},\uparrow} \right) + \left(-t c^\dagger_{\vec{R}',\uparrow} c_{\vec{R},\uparrow} \right) \left(-t c^\dagger_{\vec{R},\downarrow} c_{\vec{R}',\downarrow} \right) \right] | \, \sigma_{\vec{R}}, \bar{\sigma}_{\vec{R}'} \, \rangle \\
&= t^2 \left(c^\dagger_{\vec{R},\downarrow} c_{\vec{R},\uparrow} c_{\vec{R}',\downarrow} c^\dagger_{\vec{R}',\uparrow} + c_{\vec{R},\uparrow} c^\dagger_{\vec{R},\downarrow} c^\dagger_{\vec{R}',\uparrow} c_{\vec{R}',\downarrow} \right) | \, \sigma_{\vec{R}}, \bar{\sigma}_{\vec{R}'} \, \rangle \\
&= -2t^2 c^\dagger_{\vec{R},\downarrow} c_{\vec{R},\uparrow} c^\dagger_{\vec{R}',\uparrow} c_{\vec{R}',\downarrow} | \, \sigma_{\vec{R}}, \bar{\sigma}_{\vec{R}'} \, \rangle \\
&= -2t^2 \, | \, \bar{\sigma}_{\vec{R}}, \sigma_{\vec{R}'} \, \rangle \; .
\end{aligned} \tag{29}$$

Noticing that $S^z_{\vec{R}} = \frac{1}{2} \left[| \uparrow_{\vec{R}} \rangle \langle \uparrow_{\vec{R}} | - | \downarrow_{\vec{R}} \rangle \langle \downarrow_{\vec{R}} | \right]$, $S^+_{\vec{R}} = | \uparrow_{\vec{R}} \rangle \langle \downarrow_{\vec{R}} |$ and $S^-_{\vec{R}} = | \downarrow_{\vec{R}} \rangle \langle \uparrow_{\vec{R}} |$ we write cases (I) and (II)(a) as

$$-\frac{2t^2}{U} \left[| \uparrow_{\vec{R}}, \downarrow_{\vec{R}'} \rangle \langle \uparrow_{\vec{R}}, \downarrow_{\vec{R}'} | + | \downarrow_{\vec{R}}, \uparrow_{\vec{R}'} \rangle \langle \downarrow_{\vec{R}}, \uparrow_{\vec{R}'} | \right] = \frac{4t^2}{U} \left(S^z_{\vec{R}} S^z_{\vec{R}'} - \frac{1}{4} \right) , \tag{30}$$

and case (II)(b) as

$$\frac{2t^2}{U} \left[| \uparrow_{\vec{R}}, \downarrow_{\vec{R}'} \rangle \langle \downarrow_{\vec{R}}, \uparrow_{\vec{R}'} | + | \downarrow_{\vec{R}}, \uparrow_{\vec{R}'} \rangle \langle \uparrow_{\vec{R}}, \downarrow_{\vec{R}'} | \right] = \frac{2t^2}{U} \left(S^-_{\vec{R}} S^+_{\vec{R}'} + S^+_{\vec{R}} S^-_{\vec{R}'} \right) . \tag{31}$$

In total, summing over all n.n. we get (dropping the constant factor) the effective Hamiltonian

$$H_{\text{eff}} = J \sum_{\langle \vec{R}, \vec{R}' \rangle} \left[S^z_{\vec{R}} S^z_{\vec{R}'} + \frac{1}{2} (S^-_{\vec{R}} S^+_{\vec{R}'} + S^+_{\vec{R}} S^-_{\vec{R}'}) \right] = J \sum_{\langle \vec{R}, \vec{R}' \rangle} \vec{S}_{\vec{R}} \cdot \vec{S}_{\vec{R}'} , \tag{32}$$

with $J = \frac{4t^2}{U} > 0$, namely a Heisenberg anti-ferromagnet. Recall now that earlier in the

tutorial we truncated the interaction term

$$H_{JF} = J^F \sum_{\langle \vec{R}, \vec{R}' \rangle} c^\dagger_{\vec{R},\sigma} c^\dagger_{\vec{R}',\sigma'} c_{\vec{R},\sigma'} c_{\vec{R}',\sigma} \ , \tag{33}$$

and the $V \sum_{\langle \vec{R}, \vec{R}' \rangle} n_{\vec{R}} n_{\vec{R}'}$. The latter is trivial in the ground space, namely $P_0 n_{\vec{R}} n_{\vec{R}'} P_0 = 1$, but the former actually also gives a Heisenberg Hamiltonian

$$P_0 H_{JF} P_0 = -2 J^F \sum_{\langle \vec{R}, \vec{R}' \rangle} \vec{S}_{\vec{R}} \cdot \vec{S}_{\vec{R}'} \ . \tag{34}$$

It can be shown that for Coulomb interaction (and also for a contact interaction) $J^F > 0$, namely this interaction is ferromagnetic. Previously we could disregard it with respect to U, but now that the effective Hamiltonian (32) is of order $\frac{t^2}{U}$ the two can be comparable and should be taken together. Indeed different systems can have either one of them dominating over the other and consequently display either ferromagnetism or antiferromagnetism. This is the main mechanism by which magnetism arises in systems.

The Hubbard model can also describe BCS superconductivity. This requires changing of the sign of U from positive to negative, i.e., from repulsive to attractive. We will not dwell at this stage on how can electrons have an attractive density-density interaction (obviously Coulomb is not enough), but take this axiomatically and see how it leads to the formation of cooper pairs. Consider the following transformation on the creation and annihilation operators

$$\begin{cases} c_{\uparrow,\vec{R}} \to d_{\uparrow,\vec{R}} \\ c_{\downarrow,\vec{R}} \to (-1)^{\vec{R}} d^\dagger_{\downarrow,\vec{R}} \end{cases} \ , \tag{35}$$

where $(-1)^{\vec{R}}$ is the parity of the site at position $\vec{R}$, e.g. $(-1)^{x/a+y/a+z/a}$ on a 3d cubic lattice with unit cell of size a^3. It is easy to check that the d operators are also creation and annihilation operators, and plugging this into the Hubbard model we find

$$H_{\text{Hubbard}} = -t \sum_{\langle \vec{R}, \vec{R}' \rangle, \sigma} \left(d^\dagger_{\vec{R},\sigma} d_{\vec{R}',\sigma} + h.c. \right) - U \sum_{\vec{R}} n_{\vec{R},\uparrow} n_{\vec{R},\downarrow} \ , \tag{36}$$

namely the Hubbard model but with $U \to -U$. Performing the same transformation on the

spin operators we find

$$\begin{cases} S_{\vec{R}}^z \to n_{\vec{R}} \\ S_{\vec{R}}^+ \to (-1)^{\vec{R}} d_\uparrow^\dagger d_\downarrow^\dagger \\ S_{\vec{R}}^- \to (-1)^{\vec{R}} d_\downarrow d_\uparrow \end{cases} . \tag{37}$$

We conclude that there is a correspondence between magnetism in the repulsive Hubbard model and cooper pairs in the attractive Hubbard model. We will learn more about superconductivity later in the course.

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