Elementary Introduction to the Hubbard Model

I. INTRODUCTION

The Hubbard model offers one of the most simple ways to get insight into how the interactions between electrons can give rise to insulating, magnetic, and even novel superconducting effects in a solid. It was written down in the early 1960's and initially applied to understanding 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 Hubbard model has been applied to the understanding of many systems, from 'heavy fermion' systems in the 1980's, to high temperature superconductors in the 1990's. Indeed, it is an amazing feature of the model that, despite its simplicity, its exhibits behavior relevant to many of the most subtle and beautiful properties of solid state systems.

The Hubbard model has been studied by the full range of analytic techniques developed by condensed matter theorists, from simple mean field approaches to field theoretic methods employing Feynman diagrams, expansions in the degeneracy of the number of 'flavors' (spin, orbital angular momentum), etc. It has also been extensively attacked with numerical methods like diagonalization and quantum monte carlo.

The objective of these notes is to provide an introduction to the Hubbard model and to a few of the most simple ways in which it is solved. We begin with a discussion of the second quantized operators using which the Hubbard model is written.

II. CREATION AND DESTRUCTION OPERATORS

Creation and destruction operators $a^\dagger, a$ are familiar from the treatment of the harmonic oscillator. We will spend some time reviewing their properties, which parallel those of the operators in the Hubbard model in many ways, in this more familiar setting. The harmonic oscillator creation and destruction operators are defined in terms of the position and momentum operators,

$$\begin{aligned} \hat{a} &= \sqrt{\tfrac{m\omega}{2\hbar}}\ \hat{x} + i\sqrt{\tfrac{1}{2m\omega\hbar}}\ \hat{p} \\ \hat{a}^\dagger &= \sqrt{\tfrac{m\omega}{2\hbar}}\ \hat{x} - i\sqrt{\tfrac{1}{2m\omega\hbar}}\ \hat{p} \end{aligned}$$

From $[\hat{p}, \hat{x}] = -i\hbar$, it is easy to show that these operators obey the commutation relations,

$$[\hat{a}, \hat{a}^\dagger] = 1$$

and that the Hamiltonian is,

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2}).$$

The 'number operator' is defined to be $\hat{n} = \hat{a}^\dagger\hat{a}$, so that $\hat{H} = \hbar\omega(\hat{n} + \frac{1}{2})$.

Exercise 1: Verify the commutation relation $[\hat{a}, \hat{a}^\dagger] = 1$.

Exercise 2: Verify the expression for $\hat{H}$ in terms of the creation and destruction operators. Start with the usual expression for the Hamiltonian, $\hat{H} = \hat{p}^2/2m + m\omega^2\hat{x}^2/2$.

Exercise 3: Figure out the commutation relations $[\hat{n}, \hat{a}^\dagger]$ and $[\hat{n}, \hat{a}]$.

The ground state of the quantum oscillator is written as $|0\rangle$ and has the properties that,

$$\begin{aligned} \hat{a}|0\rangle &= 0 \\ \hat{H}|0\rangle &= \frac{\omega}{2}|0\rangle \end{aligned}$$

The excited states are built up by applying the creation operator repeatedly to the ground state.

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}\ |n+1\rangle$$

and obey the formula,

$$\hat{H}|n\rangle = \hbar\omega(n + \frac{1}{2})|n\rangle$$

Exercise 4a: Using the form for $\hat{H}$ in terms of the creation and destruction operators, and the commutation relations of Exercise 3, show that the state obeying $\hat{a}|0\rangle$ is indeed an eigenstate of $\hat{H}$.

Exercise 4b: Show that the state $|0\rangle$ with components $\Psi_0(x) = \langle x|0\rangle = e^{-m\omega x^2/2\hbar}$ in the position representation (that is, in the basis of eigenstates of the position operator) obeys $\hat{a}|0\rangle = 0$. Do this by using the form for $\hat{a}$ is terms of $\hat{x}$ and $\hat{p}$ and the fact that $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$ in the position basis. This helps connect the creation/destruction operator method with the wavefunctions for the eigenstates of the harmonic oscillator obtained in more conventional treatments.

Exercise 4c: Compute the wavefunctions $\Psi_1(x) = \langle x|1\rangle$ and $\Psi_2(x) = \langle x|2\rangle$ of the first two excited states of the simple harmonic oscillator by using $\Psi_0(x) = \langle x|0\rangle = e^{-m\omega x^2/2\hbar}$ and the expression for $\hat{a}^\dagger$ in terms of $\hat{x}$ and $\hat{p}$.

Exercise 5: Show that the states obtained by acting multiple times with $\hat{a}^\dagger$ on $|0\rangle$ are eigenstates of $\hat{H}$.

One often refers to $\hat{a}$ and $\hat{a}^\dagger$ as 'boson' creation and destruction operators, for reasons that are motivated by the result of Exercises 6 and 7 below. Note that henceforth I will be setting $\hbar = 1$. I will also set Boltzmann's constant $k_{\rm B} = 1$.

Exercise 6: The partition function of a quantum mechanical system is $Z = \mathrm{Tr}\, e^{-\beta\hat{H}}$. Here $\hat{H}$ is the Hamiltonian, $\beta = 1/T$ where T is the temperature, and the trace operation 'Tr' has its usual meaning as the sum of the diagonal elements. In other words, one chooses any complete set of states $|\alpha\rangle$ and then $\mathrm{Tr}\, e^{-\beta\hat{H}} = \sum_\alpha \langle\alpha|e^{-\beta\hat{H}}|\alpha\rangle$. Show that for the Harmonic

oscillator $Z = e^{-\beta\omega/2}/(1-e^{-\beta\omega})$. Use the occupation number states $|n\rangle$ as your complete set.

Exercise 7: The finite temperature expectation value of any quantum mechanical operator $\hat{A}$ is given by $\langle\hat{A}\rangle = Z^{-1}\,\mathrm{Tr}[\,\hat{A}\,e^{-\beta\hat{H}}\,]$. Show that $\langle\hat{n}\rangle = 1/(e^{-\beta\omega}-1)$, for the quantum harmonic oscillator. This is the Bose-Einstein distribution function.

The Hubbard model is written in terms of 'fermion' creation and destruction operators. These operators differ in several respects from the operators $\hat{a}^\dagger, \hat{a}$ for a single harmonic oscillator. Perhaps most confusing is a conceptual difference: the fermion operators in the Hubbard model are not introduced in terms of familiar position and momentum operators. Rather they stand on their own.

Also, instead of just one creation and one destruction operator, in the Hubbard model there is a set of such operators, which are distinguished by attaching indices $\mathbf{j}$ and σ. Thus we write $\hat{c}^\dagger_{\mathbf{j}\sigma}$ and $\hat{c}_{\mathbf{j}\sigma}$. As we shall see shortly, the index $\mathbf{j}$ labels the spatial lattice site and the index σ labels the electron spin (up or down).

As a consequence, the occupation number states are no longer characterized by a single number n, as for a single harmonic oscillator, but instead by a collection of occupation numbers $n_{\mathbf{j}\sigma}$. One writes such states as $|\, n_{\mathbf{1}\sigma}\, n_{\mathbf{2}\sigma}\, n_{\mathbf{3}\sigma}\, \ldots\, \rangle$

Because these operators are meant to describe fermions, they are defined to have certain *anticommutation* relations. (The anticommutator of two operators $\{\hat{A},\hat{B}\}$ is defined to be $\hat{A}\hat{B}+\hat{B}\hat{A}$.)

$$\begin{aligned}\{\hat{c}_{\mathbf{j}\sigma},\hat{c}^\dagger_{\mathbf{l}\sigma'}\} &= \delta_{\mathbf{j},\mathbf{l}}\delta_{\sigma,\sigma'}\\ \{\hat{c}^\dagger_{\mathbf{j}\sigma},\hat{c}^\dagger_{\mathbf{l}\sigma'}\} &= 0\\ \{\hat{c}_{\mathbf{j}\sigma},\hat{c}_{\mathbf{l}\sigma'}\} &= 0.\end{aligned}$$

An immediate consequence of these anticommutation relations is the Pauli principle: the maximum occupation of a particular site with a given spin is 1.

Exercise 8: Show that the Pauli exclusion principle is a consequence of the anticommutation relation amongst the fermion creation operators by considering $\mathbf{j} = \mathbf{i}$ and showing that $\hat{c}^\dagger_{\mathbf{j}\sigma}|1\rangle = 0$. Here $|1\rangle$ is the state with one electron on site $\mathbf{j}$ and with spin σ.

Note that while a fermion creation operator annihilates a state which already has a fermion in it, its action on the empty state is $\hat{c}^\dagger|0\rangle = |1\rangle$, which looks just like the bosonic operator $\hat{a}^\dagger$. Besides the Pauli principle, the anticommutation relations also ensure that the particles are fermions, that is, their wave function changes sign when two electrons with different labels $\mathbf{j}$ are exchanged.

Exercise 9: In Exercise 6 we showed that the partition function of $\hat{H} = \omega\hat{a}^\dagger\hat{a}$ is $Z = (1-e^{-\beta\omega})^{-1}$ (eliminating the zero point energy term). Show that the partition function of the analogous fermion Hamiltonian $\hat{H} = \epsilon\hat{c}^\dagger\hat{c}$ is $Z = (1+e^{-\beta\epsilon})$.

Exercise 10: In statistical mechanics, one can work in either an ensemble of fixed particle number, or one in which the particle number is allowed to vary, controlled by the chemical potential μ. More precisely, the term $-\mu\hat{N}$ is added to $\hat{H}$, wehere $\hat{N}$ is the total particle number. Explore this idea within the context of the preceding problem by considering $\hat{H} = (\epsilon-\mu)\hat{c}^\dagger\hat{c}$. Plot $\langle\hat{n}\rangle$ as a function of μ for different values of β.

Because of the anticommutation relation of the fermion operators, one needs to specify a convention for the relation between a state like $|\,1\,0\,1\,0\,0\,\ldots\rangle$ and the vacuum state $|\mathrm{vac}\rangle = |\,0\,0\,0\,0\,0\,\ldots\rangle$. The two possibilities, $|\,1\,0\,1\,0\,0\,\ldots\rangle = c^\dagger_{\mathbf{1}} c^\dagger_{\mathbf{3}} |\mathrm{vac}\rangle$ and $|\,1\,0\,1\,0\,0\,\ldots\rangle = c^\dagger_{\mathbf{3}} c^\dagger_{\mathbf{1}} |\mathrm{vac}\rangle$ differ by a sign. Either definition is fine, but in all subsequent manipulations whatever convention was chosen must be followed consistently.

Exercise 11: Suppose the index labeling the fermion operators runs over eight possible values. Figure out the occupation number state which results from the following applications of the indicated creation and destruction operators. Choose as your convention that a given occupation number state is formed by acting on the vacuum state with the lowest indices at the right of the string of creation operators. (This corresponds to the second of the two choices discussed above.)

$$\hat{c}^\dagger_5\, \hat{c}^\dagger_4\, \hat{c}^\dagger_2\, |\mathrm{vac}\rangle = ?$$
$$\hat{c}^\dagger_2\, \hat{c}^\dagger_4\, \hat{c}^\dagger_5\, |\mathrm{vac}\rangle = ?$$
$$\hat{c}^\dagger_4\, \hat{c}^\dagger_5\, |\,1\,1\,0\,0\,0\,0\,0\,1\,\rangle = ?$$
$$\hat{c}^\dagger_4\, \hat{c}^\dagger_5\, |\,1\,1\,0\,0\,1\,0\,0\,1\,\rangle = ?$$
$$\hat{c}^\dagger_1\, \hat{c}_2\, |\,0\,1\,0\,0\,1\,0\,0\,1\,\rangle = ?$$
$$\hat{c}^\dagger_1\, \hat{c}_4\, |\,0\,1\,0\,0\,1\,0\,0\,1\,\rangle = ?$$
$$\hat{c}^\dagger_1\, \hat{c}_5\, |\,0\,1\,0\,0\,1\,0\,0\,1\,\rangle = ?$$

III. THE HUBBARD HAMILTONIAN

Having introduced creation and annihilation operators, we can now write down the Hubbard Hamiltonian. Before doing so, let's think about how we might simply describe the motion and interactions of electrons in a solid.

First, we need to account for the fact that there is a regular array of nuclear positions in a solid, which for simplicity we consider to be fixed. (In other words, we will not worry about lattice vibrations.) This suggests that we begin with a lattice of atoms (sites) on which the electrons move. A single atom is already a very complex structure, with many different energy levels. The most simple 'atom' we can imagine would have a single energy level. Then, the Pauli principle would tell us that at most two electrons (one with spin up and one with spin down) can sit on this 'atom'.

In a solid where electrons can move around, the electrons interact via a screened Coulomb interaction. The biggest interaction will be for two electrons on the same atom. For simplicity, Hubbard stops just there, so that interactions are modeled by a term which is zero if the atom is empty of electrons or has only a single electron on it, but has the value U if the atom has two electrons. There is no interaction between electrons on different sites.

Our kinetic energy will consist of an expression which allows electrons to move from one site to its neighbors. The energy scale t which governs this 'hopping' will be determined by the overlap of two wavefunctions on the pair of atoms. Since wavefunctions die off exponentially, we can begin by allowing hopping only between the closest atoms in our lattice.

Now let's formalize this construction. We define $c^\dagger_{\mathbf{j}\sigma}$ to be the operator which creates an electron of spin σ on lattice site $\mathbf{j}$. (We will now drop all the 'hats' which I had been

using to emphasize things were operators.) Similarly, $c_{\mathbf{j}\sigma}$ is the destruction operator, and $n_{\mathbf{j}\sigma} = c^\dagger_{\mathbf{j}\sigma} c_{\mathbf{j}\sigma}$ is the number operator.

The Hubbard Hamiltonian is then,

$$H = -t \sum_{\langle \mathbf{j},\mathbf{l}\rangle \sigma} c^\dagger_{\mathbf{j}\sigma} c_{\mathbf{l}\sigma} + U \sum_{\mathbf{j}} n_{\mathbf{j}\uparrow} n_{\mathbf{j}\downarrow} - \mu \sum_{\mathbf{j}} (n_{\mathbf{j}\uparrow} + n_{\mathbf{j}\downarrow}).$$

The first term is the kinetic energy: It describes the destruction of an electron of spin σ on site $\mathbf{l}$ and its creation on site $\mathbf{j}$ (or *vice-versa*). The symbol $\langle \mathbf{j}, \mathbf{l}\rangle$ emphasizes that hopping is allowed only between two sites which are adjacent. The second term is the interaction energy. It goes through all the sites and adds an energy U if it finds that the site is doubly occupied. The final term is a chemical potential which controls the filling. (See Exercise 10.) We refer to the situation where the filling is one electron per site as 'half-filling' since the lattice contains half as many electrons as the maximum number (two per site). Studies of the Hubbard model often focus on the half-filled case because it exhibits a lot of interesting phenomena (Mott insulating behavior, anti-ferromagnetic order, etc.)

IV. ONE SITE

We can get a first insight into the Hubbard model by considering just a single site. Alternately phrased, we can set $t = 0$ in the Hamiltonian, in which case we have a collection of independent sites. The one site model is easily solved. We have four possibilities corresponding to the site being empty, having a single electron (either spin up or spin down) or being doubly occupied. Each of the states $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$ is an eigenstate of H with eigenvalues $0, -\mu, -\mu, U - 2\mu$ respectively. The partition function is

$$Z = \sum_\alpha \langle \alpha | e^{-\beta H} | \alpha \rangle = 1 + 2e^{\beta\mu} + e^{2\beta\mu - \beta U},$$

and the energy is,

$$E = \langle H + \mu n \rangle = Z^{-1} \sum_\alpha \langle \alpha | H e^{-\beta H} | \alpha \rangle = (1 + 2e^{\beta\mu} + e^{2\beta\mu - \beta U})^{-1} \, U \, e^{2\beta\mu - \beta U}.$$

Exercise 12: Show that the occupation is given by,

$$\rho = \langle n \rangle \quad = 2(1 + 2e^{\beta\mu} + e^{2\beta\mu - \beta U})^{-1} (e^{\beta\mu} + e^{2\beta\mu - \beta U})$$

Plot ρ vs. μ for $U = 4$ and $T = 2$. Plot ρ vs. μ for $U = 4$ and $T = 0.5$.

The plots of ρ versus μ you made in Exercise 12 exhibit some of the fundamental physics of the Hubbard model, namely the "Mott insulating gap". This will be discussed in more detail in Section IX, but for now, consider the following: at $T = 0$ the chemical potential μ has the property that $\mu = \partial E / \partial \rho$. In words, μ tells you how much the energy changes when you change the density of the system. If you have a noninteracting system described by a set of energy levels, and you have filled the levels up to some 'Fermi energy' E_F the cost to add a particle is the next energy level just above the last level you filled, that is, $\mu = E_F$.

If you reach a gap, a region of energy where there are no further levels to be filled, then μ has to take a jump from the energy at the top of the band which has just been filled to the energy at the bottom of the next band. Thus a jump in μ reflects the existence of a

gap (and hence that your system is insulating). It turns out that even when interactions are turned on, and you cannot describe the system in terms of a bunch of energy levels, a jump in μ still indicates the existence of a gapped, insulating phase.

In Exercise 12 you found that at low temperature ($T = 0.5$) μ jumps suddenly to a higher value when the filling crosses through $\rho = 1$. This is the most simple indication of a 'Mott' insulating phase in the half-filled Hubbard model.

Exercise 13: Show that $E - \mu\rho = -\partial \ln Z/\partial\beta$. Can you show this is true generally, for any H?

In Exercise 12 you should have found that you are at half-filling $\rho = 1$ when $\mu = U/2$. Because half-filling is so often studied, it is convenient to write the Hubbard Hamiltonian as,

$$H = -t \sum_{\langle \mathbf{j},\mathbf{l}\rangle\sigma} c^{\dagger}_{\mathbf{j}\sigma} c_{\mathbf{l}\sigma} + U \sum_{\mathbf{j}} (n_{\mathbf{j}\uparrow} - \frac{1}{2})(n_{\mathbf{j}\downarrow} - \frac{1}{2}) - \mu \sum_{\mathbf{j}} (n_{\mathbf{j}\uparrow} + n_{\mathbf{j}\downarrow})$$

This just corresponds to a shift in the chemical potential μ by $U/2$. When this is done, half-filling conveniently occurs always at $\mu = 0$ for any value of t, T, U. To emphasize, the properties of this 'new' model are identical to the old one, if one compares them at the same density. It's just that the chemical potentials used to get those densities are offset.

Exercise 14: Write expressions for Z, E and ρ with this new convention for the interaction term in the Hubbard model. You should notice that they are a bit more symmetric looking at $\mu = 0$.

Exercise 15: Make a plot of the energy $E = \langle H \rangle$ and the specific heat $C = dE/dT$ at half-filling as a function of T for $U = 4$.

A fundamental physical quantity in the Hubbard model is the 'local moment'. Formally, this quantity is defined by,

$$\langle m^2 \rangle = \langle (n_\uparrow - n_\downarrow)^2 \rangle.$$

In words, the local moment is zero if the site is either empty ($|0\rangle$) or has two oppositely pointed spins ($|\uparrow\downarrow\rangle$), but takes the value one if the site has a single electron ($|\uparrow\rangle$ or $|\downarrow\rangle$). The following Exercise is of great importance. What you will see is that as U increases or as T decreases, local moments form. This is our first hint concerning the magnetic properties of the Hubbard model.

Exercise 16: Make a plot of the local moment as a function of U at half-filling for fixed $T = 2$. Make a plot of the local moment as a function of T at half-filling for fixed $U = 4$. By considering the four different possible configurations of a site, explain why at high temperatures the local moment takes on the value $\langle m^2 \rangle = \frac{1}{2}$. Similarly, explain physically why $\langle m^2 \rangle = 1$ at low temperatures or large values of U.

Exercise 17: Show the local moment is related to the 'double occupancy' $d = \langle n_\uparrow n_\downarrow \rangle$ by,

$$\langle m^2 \rangle = \langle n_\uparrow + n_\downarrow \rangle - 2d.$$

(You'll need to use $n_\sigma^2 = n_\sigma$. Why is that true?) At half-filling, the relation between the moment and the double occupancy becomes $\langle m^2 \rangle = 1 - 2d$. In this case, interpret the evolution of the local moment between the two limits $\langle m^2 \rangle = \frac{1}{2}$ and $\langle m^2 \rangle = 1$ in terms of what the double occupancy d is doing.

V. ONE ELECTRON SECTOR

We begin with an Exercise.

Exercise 18: Show that the Hubbard Hamiltonian commutes with the operators $N_\uparrow = \sum_{\mathbf{j}} n_{\mathbf{j}\uparrow}$ and $N_\downarrow = \sum_{\mathbf{j}} n_{\mathbf{j}\downarrow}$. It is useful to begin by considering the commutator of the kinetic energy on a single 'link' of the lattice connecting sites **i** and **j** with the total number of electrons on those two sites. That is, begin by computing,

$$[c^\dagger_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + c^\dagger_{\mathbf{j}\sigma} c_{\mathbf{i}\sigma}, n_{\mathbf{i}\sigma} + n_{\mathbf{j}\sigma}]$$

After working through the algebra, can you think of an argument that this should be the case based on the structure of H, that is, based on how the creation and destruction operators appear together?

The implication of this Exercise is that in finding the eigenstates of the Hubbard model, we can consider different sectors of $N_\uparrow$ and $N_\downarrow$ separately. So let's consider the sector where $N_\uparrow = 1$ and $N_\downarrow = 0$.

Exercise 19: The general rule for the eigenvalues of an NxN tridiagonal matrix with "a" along the diagonal and "b" above and below the diagonal, with periodic boundary conditions, is $\lambda_n = a + 2b\cos k_n$ where $k_n = 2\pi n/N$ and $n = 1, 2, 3, \ldots N$. Show this result is correct for a 4x4 matrix. For general N, what is the eigenvector corresponding to $n = N$? What is the eigenvector corresponding to $n = N/2$?

Exercise 20: Suppose you have a one dimensional lattice of eight sites. Write all the states in this sector down. Figure out what H does to each state. Use 'periodic boundary conditions' so that site eight is considered a neighbor of site one. Write down the 8x8 matrix for H. Determine the eigenvalues (using the result of the preceding Exercise).

VI. LIMIT OF NO INTERACTIONS

We just finished looking at the single site limit, $t = 0$. The other extreme of the Hubbard model is obtained by setting $U = 0$. In the absence of interactions, it is convenient to transform operators to momentum space by defining,

$$c^\dagger_{\mathbf{k}\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{l}} e^{i\mathbf{k}\cdot\mathbf{l}} c^\dagger_{\mathbf{l}\sigma}.$$

You can think about this process in analogy with the classical normal mode problem: You are defining new (moemtum) creation operators as a linear combination of the old (position) ones. As we shall see in Exercises 23 and 24, for the Hubbard model at $U = 0$ the different

momentum modes decouple from each other and behave independently, just as for classical normal modes.

Notice that on a finite lattice the momentum $\mathbf{k}$ cannot be any real number but has discretized values. For a one-dimensional lattice of N sites, $k_n = 2\pi n/N$, if periodic boundary conditions are employed. For a two-dimensional square or three dimensional cubic lattice, each component separately has such a discretization. These quantized momentum values come from the identification of site $N+1$ with site 1, thereby requiring that kN be an integer muliple of 2π.

You know that the different Fourier functions are orthogonal. The analog for these discrete site and momentum variables is given in the following Exercise:

Exercise 21: Prove the following two 'orthogonality' relations:

$$\begin{aligned} \frac{1}{N}\sum_{l} e^{i(k_n - k_m)l} &= \delta_{n,m} \\ \frac{1}{N}\sum_{n} e^{ik_n(l-j)} &= \delta_{l,j} \end{aligned}$$

Exercise 22: Use the orthogonality relations to prove,

$$c^\dagger_{\mathbf{l}\sigma} = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{l}} c^\dagger_{\mathbf{k}\sigma}.$$

Here, of course, the sum over $\mathbf{k}$ means you sum over the discrete allowed momenta $\mathbf{k}_n$. With these relations in hand, we can show a lot of interesting things about the momentum space operators.

Exercise 23: Verify that anticommutation relations

$$\begin{aligned} \{c_{\mathbf{k}\sigma}, c^\dagger_{\mathbf{p}\sigma'}\} &= \delta_{\mathbf{k},\mathbf{p}}\delta_{\sigma,\sigma'} \\ \{c^\dagger_{\mathbf{k}\sigma}, c^\dagger_{\mathbf{p}\sigma'}\} &= 0 \\ \{c_{\mathbf{k}\sigma}, c_{\mathbf{p}\sigma'}\} &= 0. \end{aligned}$$

In other words, the anticommutation relations are "preserved" by this change in "basis" from site indices to momentum indices.

We can now write down the $U = 0$ Hubbard model in terms of these momentum space operators.

Exercise 24: Show that for $U = 0$ the one dimensional Hubbard model is,

$$H = \sum_{k\sigma} (\epsilon_k - \mu) c^\dagger_{k\sigma} c_{k\sigma}$$

where $\epsilon_k = -2t\cos k$. As part of this Exercise, you will show that the sum of all the number operators over different spatial sites and spin equals the sum of all the number operators over different momenta and spin. Is this reasonable?

This Hamiltonian looks like the one arising in the quantum oscillator in the sense that it is expressed in terms of independent number operators. Note also that this is precisely the dispersion relation which we obtained when we looked at the one particle sector in Exercises (18-19) of the preceding section. For $U = 0$ looking at the one particle sector, as we did earlier, tells us everything about all the particle sectors: At $U = 0$, even if one has many particles, they just occupy the one particle states in accordance with the Pauli principle. When U is non-zero, however, the one particle sector eigenenergies do not tell us much about the energies of the sectors with more particles.

It is important to realize that the result that an analysis of the one-particle sector gives us full information about the model for any particle number rests only on the fact that the interactions are turned off. It is not necessary that the hopping t between different sites be the same for all pairs of sites, or that it be limited to near neighbors, or that the chemical potential be the same on all sites. All that matters is that H be a quadratic form in the fermion creation and destruction operators. To emphasize: To solve any Hamiltonian H which takes the form $H = \sum_{\mathbf{i},\mathbf{j}} c^\dagger_{\mathbf{i}} h_{\mathbf{i},\mathbf{j}} c_{\mathbf{j}}$ with h a (symmetric) matrix of real numbers, simply diagonalize h and allow the resulting energy levels to be filled in a way which satisfies the exclusion principle. We will see an important application of this theorem when we do mean field theory.

Exercise 25: Show that for $U = 0$ the two dimensional Hubbard model on a square lattice is

$$H = \sum_{\mathbf{k}\sigma} (\epsilon_{\mathbf{k}} - \mu) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

where $\epsilon_{\mathbf{k}} = -2t\,(\cos k_x + \cos k_y)$.

What have we accomplished? In real space, all the different sites in the $U = 0$ model are mixed with each other: If you start an electron off on a given site, it will not remain there. The kinetic energy will move it to adjacent sites. But in momentum space the different modes are decoupled: A fermion operator of a give $\mathbf{k}$ appears only together with operators of the same $\mathbf{k}$. This means that the different momentum modes can be treated independently, leading to the result in the following Exercise.

Exercise 26: Show that the partition function of the $U = 0$ Hubbard model is given by

$$Z = \prod_{\mathbf{k}} (1 + e^{-\beta(\epsilon_{\mathbf{k}} - \mu)}).$$

This is the generalization of Exercise 9 to many independent modes. It is useful to remember that if a Hamiltonian is comprised of the sum of independent pieces then the partition function is the product of the associated partition functions. Can you prove this? The result is also true for classical systems.

Exercise 27: Compute the per site average occupation of the $U = 0$ Hubbard model and show it is given by,

$$\rho = \sum_{\mathbf{k}} (1 + e^{+\beta(\epsilon_{\mathbf{k}} - \mu)})^{-1}.$$

Note this takes the form of the sum of the occupations of different pieces, and that the Fermi function, $f_{\mathbf{k}} = 1/[1 + e^{\beta(\epsilon_\sigma(k) - \mu)}]$, naturally arises.

Exercise 28: Compute the average energy of the $U = 0$ Hubbard model and show it is given by,

$$E = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} (1 + e^{+\beta(\epsilon_{\mathbf{k}} - \mu)})^{-1}.$$

Again, this takes the form of the sum of the energies of different pieces.

Exercise 29: Make a graph of E vs T for $t = 1$ and half-filling ($\mu = 0$).

Much of this discussion also has analogues with the introduction of normal modes in classical mechanics, where the goal is similarly to eliminate a set of degrees of freedom which couple to each other in favor of ones which do not.

The allowed k values together with the dispersion relation determine the density of states $N(E)$ which counts the number of ways in which the system can have a given energy E. Formally, $N(E)$ is defined by

$$N(E) = \frac{1}{N} \sum_{\mathbf{k}} \delta(E - \epsilon_{\mathbf{k}}).$$

In the continuum limit (large number of sites) the sum over discrete momenta values is replaced by an integral according to the rule $\frac{1}{N} \sum_{\mathbf{k}} \rightarrow (2\pi)^{-d} \int d\mathbf{k}$, where d is the spatial dimension. As a simple example, suppose we are in one dimension with a relativistic dispersion relation $\epsilon_k = ck$ for $k > 0$. We can get the density of states as follows:

$$N(E) = (2\pi)^{-1} \int dk \delta(E - ck) = (2\pi)^{-1} \int dk \frac{1}{c} \delta(E/c - k) = (2c\pi)^{-1} (1 - \theta(k)).$$

Here the function $1 - \theta(k)$ emphasizes that $k > 0$ is required. Likewise, for a quadratic dispersion relation $\epsilon_k = ak^2$

$$N(E) = (2\pi)^{-1} \int dk \delta(E - ak^2) = (2\pi)^{-1} \int dk \frac{1}{2ak} \delta(\sqrt{E/a} - k) = (4a\pi)^{-1} \sqrt{a/E}.$$

Exercise 30: Compute (analytically) the density of states $N(E)$ of one dimensional Hubbard model. You will need to remember how to deal with the δ function of a function $f(x)$, a simple example of which occurred above in the calculation of the density of states for a quadratic dispersion. Explain why $N(E)$ diverges at $E = \pm 2t$ in terms of a picture of the dispersion relation $E(k) = -2t \cos k$. Compute $N(E)$ numerically and compare to your analytic calculation.

Exercise 31: Compute (numerically) the density of states $N(E)$ of the two dimensional square lattice Hubbard model which has

$$\epsilon_{k_x, k_y} = -2t(\cos k_x + \cos k_y).$$

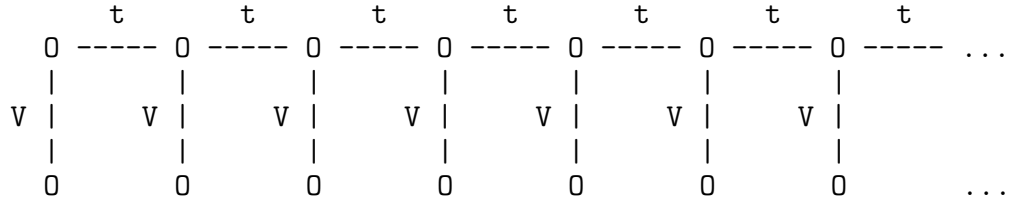
Show the $N(E = 0)$ diverges. Can you compute $N(E)$ analytically? Comment: There are a number of physical responses of a system which have a temperature scale $T_* = V_1 e^{-1/(N(E_F)V_2)}$ where V_1 and V_2 are some energy scales in the problem and E_F is the Fermi energy. If $N(E_F)$ diverges, T_* can be large. This was suggested as possibly playing a role in the origin of high temperature superconductivity.

Exercise 32: Compute (numerically) the density of states $N(E)$ of the Hubbard model on a two dimensional honeycomb lattice. You will need first to figure out the dispersion relation. You should find that $N(E)$ vanishes linearly at $E = 0$. The system is said to be a semi-metal there. You will need to figure out how the periodic boundary conditions restricts the allowed $\mathbf{k}$ values.

Exercise 33: Compute (numerically) the density of states $N(E)$ of the Hubbard model on a two dimensional triangular lattice. You will need first to figure out the dispersion relation. Unlike all the preceding cases, you will find that $N(E) \neq N(-E)$. This is a consequence of the fact that the model is not "particle-hole" symmetric on a triangular lattice. This will be discussed further below. As in the preceding Exercise, you will need to figure out how the periodic boundary conditions restricts the allowed $\mathbf{k}$ values.

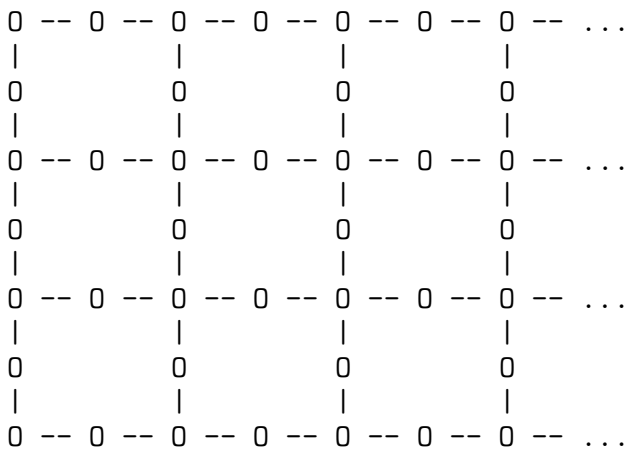
Actually, there are some more commonly occuring lattice structures in model Hamiltonians whose dispersion relation you might want to work out. They are discussed in the following two Exercises:

Exercise 34: A model almost as widely studied as the Hubbard Hamiltonian is the 'Periodic Anderson Model' (PAM). It consists first of a set of sites whose near neighbors are connected with hopping 't'. These might be in a one-d chain, or a two-d square lattice arrangement for example. Then there is a second set of sites in the same geometry, except they are disconnected from each other. The electrons cannot hop between these sites. However, an electron on one of these second set of sites can hop to their partners in the first set with energy 'V'. In d=1 one might have the following picture:



Compute $E(k)$ and $N(E)$ for this model. Compare what happens at $V = 0$ with $V \neq 0$. Do the words 'level repulsion' enter your discussion? How about 'energy gap'? The physics this model is attempting to describe is that of a set of 'conduction electrons' which can hop from site to site and a set of 'localized electrons' which cannot move from site to site, but which can move into the conduction orbital on the same site. If one adds a Hubbard U on the localized orbitals one gets the Periodic Anderson model.

Exercise 35: A three-band Hubbard model widely studied for high temperature superconductivity has the geometry:



Compute $E(k)$ and $N(E)$. Does one of your bands have a very simple form? This geometry can be viewed as a square array of sites with additional sites sitting on the links between them. The copper atoms in high-T_c materials form just such a planar square arrays, whilst the oxygen atoms sit between them.

VII. GREENS FUNCTION: DEFINITION AND EXAMPLES FOR $U = 0$

The one particle Greens function,

$$G_{\mathbf{ln}}(\tau) = \langle c_{\mathbf{l}}(\tau) c^{\dagger}_{\mathbf{n}}(0) \rangle$$
$$c_{\mathbf{l}}(\tau) = e^{H\tau} c_{\mathbf{l}}(0) e^{-H\tau},$$

is a fundamental quantity in understanding the many body physics of interacting electron systems. Its momentum space and frequency transform yields the photoemission spectrum, and from it two particle Greens functions which yield the charge and spin susceptibilities can be obtained.

In the limit of no interactions, $G_{\mathbf{ln}}(\tau)$ can be computed analytically.

Exercise 36: Show that at $U = 0$,

$$c_{\mathbf{k}}(\tau) = e^{H\tau} c_{\mathbf{k}}(0) e^{-H\tau} = e^{-\epsilon_{\mathbf{k}}\tau} c_{\mathbf{k}}(0)$$

You should do this two ways: First show that both expressions give the same result on the two states $|0\rangle$ and $|1\rangle$. Next, prove the result using the general theorem that $\partial A(\tau)\partial\tau = [H, A(\tau)]$. (This result immediately follows from the definition $A(\tau) = e^{H\tau} A(0) E^{-H\tau}$.)

Exercise 37: Show that at $U = 0$,

$$G_{\mathbf{ln}}(\tau) = \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{n}-\mathbf{l})} (1 - f_{\mathbf{k}}) e^{-\epsilon_{\mathbf{k}}\tau}.$$

Notice that G is just a function of the difference $\mathbf{n} - \mathbf{l}$, as you would expect for a translationally invariant Hamiltonian.

Exercise 38: Write a program to evaluate $G_{\mathbf{ln}}(\tau)$ numerically at $U = 0$ for a $d = 1$ chain and a $d = 2$ square lattice.

Actually, we have been a little bit sloppy in defining G. Usually in many-body theory one defines the so-called 'time ordered' Green's function, $G_{\mathbf{k}}(\tau) = -\langle \mathcal{T} c_{\mathbf{k}}(\tau) c_{\mathbf{k}}(0) \rangle$ where the time ordering operator T is defined by

$$\begin{aligned} \mathcal{T} c_{\mathbf{k}}(\tau) c_{\mathbf{k}}(0) &= c_{\mathbf{k}}(\tau) c_{\mathbf{k}}(0) & \tau > 0 \\ \mathcal{T} c_{\mathbf{k}}(\tau) c_{\mathbf{k}}(0) &= -c_{\mathbf{k}}(0) c_{\mathbf{k}}(\tau) & \tau < 0 \end{aligned}$$

This definition of G opens the door into the huge world of diagrammatic perturbation theory and its application to the Hubbard model, an immense field that we cannot hope to address. However, the next few Exercises take you down the road just a little way.

Exercise 39: Prove that $G(\tau + \beta) = -G(\tau)$ for $-\beta < \tau < 0$.

Exercise 40: Prove that the result of Exercise (39) requires that the Fourier transform of G given by

$$G(\tau) = \sum_n G(i\,\omega_n) e^{-i\omega_n \tau}$$

employs the 'Matsubara frequencies' $\omega_n = \pi(2n+1)/\beta$.

Exercise 41: Prove the inversion relation

$$G(i\,\omega_n) = \int_0^\beta \frac{d\tau}{\beta} G(\tau) e^{i\,\omega_n \tau}$$

Exercise 42: In Exercise (36) we solved for the time evolution of the fermion operator for $H = \epsilon_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}}$. Show that the Greens function is given by

$$\begin{aligned} G_{\mathbf{k}}(\tau) &= -e^{-\epsilon_{\mathbf{k}}\tau}(1 - f_{\mathbf{k}}) & 0 < \tau < \beta \\ G_{\mathbf{k}}(\tau) &= e^{-\epsilon_{\mathbf{k}}\tau} f_{\mathbf{k}} & -\beta < \tau < 0 \end{aligned}$$

Exercise 43: Using the result of Exercise (42) and the transformation rule of Exercise (41) show that

$$G_{\mathbf{k}}(i\,\omega_n) = \frac{1}{i\,\omega_n - \epsilon_{\mathbf{k}}}.$$

Exercise 44: Another way to get the result of Exercise (43) is to take $\partial/\partial\tau$ of the definition of the time ordered Greens function written in the form

$$G_{\mathbf{k}}(\tau) = \langle c_{\mathbf{k}}(\tau) c_{\mathbf{k}}(0) \rangle\, \theta(\tau) - \langle c_{\mathbf{k}}(0) c_{\mathbf{k}}(\tau) \rangle\, \theta(-\tau).$$

Be careful to take the appropriate derivatives of the step functions! Then Fourier transform both sides and solve for $G_{\mathbf{k}}(i\,\omega_n)$. Show that this indeed reproduces Exercise (43).

The approach used in Exercise (44) is the basis of the 'equation of motion' method for computing G. One starts with the definition of G, takes a time derivative, evaluates the resulting commutators of H with c and then Fourier transforms. If the Hamiltonian is quadratic in the fermion operators, then the set of equations so obtained closes, even if the different fermion operators mix.

Exercise 45: The ambitious student should use the above procedure to evaluate $G_{\mathbf{k}}(i\,\omega_n)$ and $G_d(i\,\omega_n)$ for

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}} c_{\mathbf{k}} + V \sum_{\mathbf{k}} (c^\dagger_{\mathbf{k}} d + d^\dagger c_{\mathbf{k}}) + \epsilon_d d^\dagger d$$

which describes the mixing of a single impurity orbital (labeled by 'd') with a band of conduction electrons (labeled by '$\mathbf{k}$'). You will need to write the two definitions of $G_{\mathbf{k}}(\tau)$ and $G_d(\tau)$, take their τ derivatives, and Fourier transform. You'll end up with two equations in two unknowns (the two Greens functions). Solving, your result for G_d should be

$$G_d(i\,\omega_n) = -\frac{1}{i\,\omega_n - \epsilon_d - V^2 \sum_{\mathbf{k}} \frac{1}{i\,\omega_n - \epsilon_{\mathbf{k}}}}$$

VIII. GREENS FUNCTION: $t = 0$

It is also instructive to look at the Green's function for a single site, that is, the $t = 0$ Hubbard model. We have previously written down the Hilbert space for this problem and obtained the partition function and various equal time quantities. Now consider the calculation of

$$G_\uparrow(\tau) = \langle c_\uparrow(\tau) c^\dagger_\uparrow(0) \rangle.$$

Only the states $|\,0\,0\,\rangle$ and $|\,0\,1\,\rangle$ contribute to the expectation value since the creation operator for up electrons needs to see an empty up state. We can easily compute the action of the sequence of operators on $|\,0\,0\,\rangle$:

$$\begin{aligned} c_\uparrow(\tau) c^\dagger_\uparrow(0)\ |\,0\,0\,\rangle &= e^{H\tau} c_\uparrow(0) e^{-H\tau} c^\dagger_\uparrow(0)\ |\,0\,0\,\rangle = e^{H\tau} c_\uparrow(0) e^{-H\tau}\ |\,1\,0\,\rangle \\ &= e^{H\tau} c_\uparrow(0) e^{+U\tau/4}\ |\,1\,0\,\rangle = e^{H\tau} e^{+U\tau/4}\ |\,0\,0\,\rangle = e^{+U\tau/2}\ |\,0\,0\,\rangle \end{aligned}$$

and similarly for $|\,0\,1\,\rangle$.

Exercise 46: Complete the calculation begun above to show that,

$$G_\uparrow(\tau) = \frac{e^{+\beta U/4} e^{-\tau U/2} + e^{-\beta U/4} e^{\tau U/2}}{2\,e^{\beta U/4} + 2\,e^{-\beta U/4}}.$$

Exercise 47: The Green's function is related to the spectral density $A(\omega)$ by the relation,

$$G(\tau) = \int_{-\infty}^{+\infty} A(\omega) \frac{e^{-\omega\tau}}{e^{-\beta\omega} + 1}\, d\omega.$$

Show that if you plug in

$$A(\omega) = \frac{1}{2}\ (\ \delta(\omega - U/2) + \delta(\omega + U/2)\ )$$

and do the integral you get precisely the $G(\tau)$ we computed.

This is one way (there are others) to show that the spectral function in Hubbard-1 consists of two delta function peaks separated by U (the Mott gap).

It is also interesting to compute G and A when there is a local site energy or chemical potential present. To this end, we work with the Hamiltonian $H = U(n_\uparrow - \frac{1}{2})(n_\downarrow - \frac{1}{2}) - \mu(n_\uparrow + n_\downarrow)$, Your first guess might be that,

$$A(\omega) = \frac{1}{2}\ (\ \ \delta(\omega - U/2 + \mu) + \delta(\omega + U/2 + \mu)\ \ ).$$

The logic behind this guess is that the Hamiltonian now contains an on-site energy term (the chemical potential) which seems like it should just shift all the energies ω down by μ. But this is not right! The pole positions are correct, but the weights of the poles are no longer equal.

Exercise 48: Show that the correct result is,

$$\begin{aligned} A(\omega) &= a_+\ \ \delta(\omega - U/2 + \mu) + a_-\ \ \delta(\omega + U/2 + \mu). \\ a_+ &= (\ e^{\beta U/2} e^{\beta\mu} + e^{2\beta\mu}\ )/(\ 1 + 2\, e^{\beta U/2} e^{\beta\mu} + e^{2\beta\mu}) \\ a_- &= (\ 1 + e^{\beta U/2} e^{\beta\mu}\ )/(\ 1 + 2\, e^{\beta U/2} e^{\beta\mu} + e^{2\beta\mu}\ ) \end{aligned}$$

by evaluating $G(\tau)$ explicitly from its definition. μ now enters both the partition function Z and the imaginary time propagation. The coefficients a_+ and a_- are obtained by equating this expression for $G(\tau)$ with what you get from plugging $A(\omega)$ into the formula relating G and A. Notice that at $\mu = 0$ we recover $a_+ = a_- = \frac{1}{2}$, and that, regardless of what μ, β and μ are, we always have $a_+ + a_- = 1$.

IX. INTERACTION TERM IN MOMENTUM SPACE

Even though we will not pursue this line of approach, it is interesting to write down the interaction term in momentum space.

Exercise 49: Substitute the equation which relates real and momentum space operators for each of the four real space creation operators in the interaction term of the Hubbard model. As with the hooping term, the sum over sites leads to momentum conservation and reduces the four momentum sums to three. Show that the result is

$$\frac{U}{N} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3} c^\dagger_{\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 \uparrow} c^\dagger_{\mathbf{k}_3 \downarrow} c_{\mathbf{k}_2 \uparrow} c_{\mathbf{k}_1 \downarrow}.$$

The physical content of the this form is that an up and down electron of momentum $\mathbf{k}_2$ and $\mathbf{k}_1$ scatter and emerge with momenta $\mathbf{k}_3$ and $\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3$, the same total momentum as initially.

Actually, there are many equivalent ways to write the sum over the three momentum variables. The most elegant is probably:

$$\frac{U}{N}\sum_{\mathbf{k},\mathbf{p},\mathbf{q}} c^{\dagger}_{\mathbf{p}+\mathbf{q}\uparrow} c^{\dagger}_{\mathbf{k}-\mathbf{q}\downarrow} c_{\mathbf{p}\uparrow} c_{\mathbf{k}\downarrow}.$$

Here $\mathbf{q}$ is the momentum exchanged in the collision of the two electrons of initial momenta $\mathbf{k}$ and $\mathbf{p}$.

X. METAL-INSULATOR TRANSITIONS

We have seen the physical phenomenon of moment formation in the Hubbard model, and will discuss shortly the magnetic ordering of such moments on different sites. But first we will give a physical picture for the way in which the Hubbard Hamiltonian can describe metal-insulator transitions. The idea is simple: Imagine a half-filled lattice in which each site has one electron. In order for an electron to move, it will have to go onto a site which is already occupied. This costs an energy U. It is plausible to imagine that if U is very large, the electrons will not want to move at all, and one will have an "Mott" insulator.

The Mott insulator can be described in a slightly more subtle way which however connects a bit better with one's picture of energy gaps as giving rise to insulators. Imagine a nearly empty lattice and asking what the energy cost is to add an electron. This cost will not involve U because it is easy to find a site which is empty. When one gets to half-filling, however, suddenly the cost to add an electron jumps by U since inevitably an added electron must sit on top of an electron which is already there. This sudden jump in the cost to add a particle is referred to as the "Mott gap" and is similar in a way to the fact that the cost to add an electron jumps by some amount if there is a gap in the energy bands. It is worth noting, though, that this analogy goes only so far, and the Mott gap differs in a number of very fundamental ways from band gaps.

XI. EXACT DIAGONALIZATION

We have considered the limits $t = 0$ and $U = 0$. The Hubbard model cannot be solved exactly when both terms are non-zero. Our next approach is to consider a small cluster of sites. Let's start with two sites. The Hilbert space has 16 states, since each site can have four possibilities: no electrons, an up electron, a down electron, or both. However, since H commutes with $N_\uparrow$ and $N_\downarrow$ we actually have to consider only much smaller matrices.

Exercise 50: Show that the sixteen dimensional Hilbert space of the two site Hubbard model factorizes into four spaces of dimension one, four spaces of dimension two, and one space of dimension four. Construct the matrices by applying H to each of the vectors.

Exercise 51: Diagonalize the matrices of the preceding Exercise. Even the four dimensional matrix can be done by hand. Compute the partition function and the energy.

Earlier, when we studied the one site Hubbard model, we learned that magnetic moments form when the ratio U/T is large. Put another way, thermal fluctuations can destroy magnetic moments, while interactions cause them to form. This was at $t = 0$. We will now see

that 'quantum fluctuations'- the motion of the electrons which occurs when the hopping t is made nonzero, also competes with moment formation.

Exercise 52: Compute the local moment $\langle m^2 \rangle$ in the sector with one up and one down electron for low temperature. Plot $\langle m^2 \rangle$ as a function of U/t. Interpret your result in terms of the effect of U and t on moment formation.

We have now learned that U drives the formation of moments on the sites of our lattice and that thermal fluctuations (T) and quantum fluctuations (t) both try to inhibit moments. We conclude this discussion of the two site case by pointing out something about the order of magnetic moments between sites in the Hubbard model.

Exercise 53: Compute the energy difference between the two states $|\uparrow\ \uparrow\rangle$ and $|\downarrow\ \downarrow\rangle$ (which have the same energy) and the lowest energy state of the sector which connects the states $|\uparrow\ \downarrow\rangle$, $|\downarrow\ \uparrow\rangle$, $|\uparrow\downarrow\ \ 0\rangle$, and $|\downarrow\uparrow\ \ 0\rangle$. Show that the lowest energy state in this $N_\uparrow = N_\downarrow = 1$ sector is lower in energy by an amount proportional to $J = t^2/U$.

The result of the preceding Exercise tells us something about magnetic order in the Hubbard model. In the half-filled sector, one elctron per site, the states with antiferromagnetic order (neighboring sites have electrons with opposite spins) are lower in energy than ferromagnetic ones (neighboring sites have parallel spins). Although this has come out of consideration of only two sites, it is a general feature: The Hubbard model has antiferromagnetic order at half-filling. Indeed, the antiferromagnetic 'exchange' energy scale $J = t^2/U$ that we found is precisely the energy scale for this order even in the thermodynamic limit.

In addition to antiferromagnetism, one can see the Mott gap in this little two site model by looking at the eigenvalues of the sector with one up and one down electron. As you found in Exercise 35, there are two eigenvalues close to $-U/2$ and two close to $+U/2$. More precisely, the eigenvalues are shifted by values involving the hopping t away from $\pm U/2$. The separation U between $\pm U/2$ is the Mott gap, and, as one increases t the separation becomes less and less clear. This puts a very simple quantitative face on the statement that when U is large one has an insulator (a Mott gap) but when U is small, the electrons can still move around.

This analysis of the two site model can be extended quite easily to somewhat larger lattices by writing a program which generates the matrix elements of H and diagonalizes the resulting matrices. In fact, this is one important way that information has been gained concerning the Hubbard model. Although it is limited to 10-20 sites (depending on how much computational effort one is willing to put up with) the results obtained are exact and any possible quantity, including time dependent ones, can be computed.

Exercise 54: Write a program to diagonalize the four site Hubbard model. Compute E and $\langle m^2 \rangle$.

In these notes, the idea of diagonalization has arisen twice. First, we pointed out that in the absence of interactions, the Hamiltonian is quadratic in the fermion creation and destruction operators, $H = \sum_{\mathbf{i},\mathbf{j}} c^\dagger_{\mathbf{i}} h_{\mathbf{i},\mathbf{j}} c_{\mathbf{j}}$, and we can solve the Hubbard model by diagonalizing the matrix h. Second, in the discussion immediately above, we talked about constructing the matrix for H when the interactions are nonzero. However, there is a very important difference in the two usages of the term "diagonalization." This is emphasized in the Exercise which follows.

Exercise 55: Compare the computational cost of the diagonalizations in each of the two cases, $U = 0$ and $U \neq 0$. How big are the matrices involved for N sites? How large a system could you study in both cases?

XII. STONER'S CRITERION FOR FERROMAGNETISM

Stoner developed a very simple picture of ferromagnetism based on the competition between the kinetic energy cost of making the up and down spin electron numbers different and the associated potential energy gain. The basic idea is the following: Because of the Pauli principle the way to occupy a given set of energy levels with the lowest energy is to start filling from the bottom and put two electrons, one of each spin, in each level. Otherwise, if you make the numbers of up and down electrons unequal, and don't fill each level with two electrons, you will have to occupy higher energies.

However, if you make the number of up and down electrons unequal, you can reduce the potential energy: Consider the limit of complete spin polarization where the are no electrons of one spin species. Then, obviously, the potential energy is zero.

Let's now make this argument more precise: Consider a system with density of states $N(E)$ and both up and down spin electrons filling the energy levels up to the same maximum called the 'Fermi level' E_F. The density of up and down electrons is equal. We'll call it n.

Let's compute the change in energy which results from a reduction in the density of down spin electrons by δn and at the same time an increase the number of up spin electrons by δn. The potential energy changes by,

$$\delta P = U(n + \delta n)(n - \delta n) - Un^2 = -U(\delta n)^2.$$

If we shift an extra δn electrons into the up group, we will occupy energy levels above the original E_F. Recalling the definition of the density of states as the number of levels at an energy E we see that $N(E) = dN/dE$ whence $\delta n = N(E_F)\delta E$. This tells us how big the range of energies is above E_F we are filling in terms of δn. Likewise, we are emptying levels below E_F that used to be occupied by down spin electrons. The net result of this process is to shift δn electrons up in energy by an amount δE. The change in the kinetic energy is then,

$$\delta K = +\delta n \delta E = +\frac{1}{N(E_F)}(\delta n)^2.$$

Putting these two expressions together,

$$\delta E = \delta P + \delta K = (-U + \frac{1}{N(E_F)})(\delta n)^2 = (-UN(E_F) + 1)\frac{(\delta n)^2}{N(E_F)}.$$

We see that if $UN(E_F) > 1$ the total energy change $\delta E < 0$, so it is favorable to have the up and down electron densities different and hence favorable to have ferromagntism. This is called the Stoner criterion. It tells us that magnetism is favored by large electron interactions.

As we shall see, this simple calculation yields results in precise agreement with mean field theory.

XIII. MEAN FIELD THEORY: FERROMAGNETISM

We have considered the Hubbard model in the simple limits of no hopping ($t = 0$), no interactions ($U = 0$), very small system sizes (one and two sites), and using Stoner's approach. We now turn to our first 'serious' calculation of the Hubbard model- mean field theory. Our goal is to study ferromagnetism.

What is mean field theory? We commented in an earlier section that a Hamiltonian which is quadratic in the fermion creation and destruction operators, $H = \sum_{\mathbf{i},\mathbf{j}} c^\dagger_{\mathbf{i}} h_{\mathbf{i},\mathbf{j}} c_{\mathbf{j}}$, can be solved by diagonalizing the matrix h. Mean field theory is a method which produces such a quadratic Hamiltonian from a model like the Hubbard model which has quartic terms $U c^\dagger_\uparrow c_\uparrow c^\dagger_\downarrow c_\downarrow$ involving four fermion creation and destruction operators. The approach begins by expressing the number operators as an average value plus a deviation from the average:

$$\begin{aligned} n_{\mathbf{i}\uparrow} &= \langle n_{\mathbf{i}\uparrow}\rangle + (n_{\mathbf{i}\uparrow} - \langle n_{\mathbf{i}\uparrow}\rangle) \\ n_{\mathbf{i}\downarrow} &= \langle n_{\mathbf{i}\downarrow}\rangle + (n_{\mathbf{i}\downarrow} - \langle n_{\mathbf{i}\downarrow}\rangle). \end{aligned}$$

Substituting these expressions into the Hubbard interaction term, and dropping the 'small' term which is the product of the two deviations from the average yields,

$$\begin{aligned} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} &= [\langle n_{\mathbf{i}\uparrow}\rangle + (n_{\mathbf{i}\uparrow} - \langle n_{\mathbf{i}\uparrow}\rangle)][\langle n_{\mathbf{i}\downarrow}\rangle + (n_{\mathbf{i}\downarrow} - \langle n_{\mathbf{i}\downarrow}\rangle)] \\ &\approx \langle n_{\mathbf{i}\uparrow}\rangle\langle n_{\mathbf{i}\downarrow}\rangle + \langle n_{\mathbf{i}\downarrow}\rangle(n_{\mathbf{i}\uparrow} - \langle n_{\mathbf{i}\uparrow}\rangle) + \langle n_{\mathbf{i}\uparrow}\rangle(n_{\mathbf{i}\downarrow} - \langle n_{\mathbf{i}\downarrow}\rangle)] \\ &= n_{\mathbf{i}\uparrow}\langle n_{\mathbf{i}\downarrow}\rangle + n_{\mathbf{i}\downarrow}\langle n_{\mathbf{i}\uparrow}\rangle) - \langle n_{\mathbf{i}\uparrow}\rangle\langle n_{\mathbf{i}\downarrow}\rangle. \end{aligned}$$

The interpretation of this expression is simple. The up spin electrons interact with the average density of down spin electrons, and similarly the down spin electrons interact with the average density of up spin electrons. These two terms overcount the original single interaction term, so the product of the average densities is subtracted off.

Within this mean field replacement, the Hubbard Hamiltonian is now quadratic, and takes the form (in one dimension)

$$H = -t\sum_{l\sigma}(c^\dagger_{l\sigma} c_{l+1\sigma} + c^\dagger_{l+1\sigma} c_{l\sigma}) + n_{\mathbf{i}\uparrow}\langle n_{\mathbf{i}\downarrow}\rangle + n_{\mathbf{i}\downarrow}\langle n_{\mathbf{i}\uparrow}\rangle) - \langle n_{\mathbf{i}\uparrow}\rangle\langle n_{\mathbf{i}\downarrow}\rangle.$$

Since H is quadratic, its solution is a matter of diagonalizing an appropriate matrix. Specifically, for the case of ferromagnetism, one imagines that the average occupation is independent of spatial site $\mathbf{i}$ but allowed to be different for the two spin species. That is, $\langle n_{\mathbf{i}\uparrow}\rangle = n+m$ and $\langle n_{\mathbf{i}\downarrow}\rangle = n - m$. Our goal is to calculate the energy E for fixed n as a function of m and see whether the minimum is at $m = 0$ (paramagnetic state, no ferromagnetism) or $m \neq 0$ (ferromagnetism). Because the expectation values $\langle n_{\mathbf{i}\uparrow}\rangle$ and $\langle n_{\mathbf{i}\downarrow}\rangle$ have such a simple, site independent form, the energy levels can easily be written down. (See Exercise 23.) They are,

$$\begin{aligned} \epsilon_{\uparrow k} &= U(n - m) - 2t\cos k \\ \epsilon_{\downarrow k} &= U(n + m) - 2t\cos k. \end{aligned}$$

Again, I have assumed we are in one dimension.

One merely has to take the various possible fillings of the lattice with up and down electrons and add these levels up. That is, we proceed as follows:

(1) Fix the lattice size, N, to some fairly large value, for example $N = 128$ or greater.

(2) Choose a total particle number $N_{\rm tot}$ and on-site repulsion U.

(3) Loop over $N_\uparrow = 0, 1, 2, \ldots . N_{\rm tot}$. For each choice, set $N_\downarrow = N_{\rm tot} - N_\uparrow$. (Actually, your answers should be symmetric on interchange of $N_\uparrow$ and $N_\downarrow$, so you really only need do half the values $N_\uparrow = 0, 1, 2, \ldots . N_{\rm tot}/2$.) Define the densities, $n_\uparrow = N_\uparrow/N$ and $n_\downarrow = N_\downarrow/N$.

(4) Loop over the N allowed momentum values $k = 2\pi/N\{-N/2+1, -N/2+2, \ldots N/2\}$. Fill up the lowest $N_\uparrow$ and $N_\downarrow$ of the energy levels. That is, add the associated energy values to some accumulator which stores the total energy. Recall that the levels are given by $\epsilon_\uparrow(k) = -2\,t\,{\rm cos}k + U\langle n_\downarrow\rangle$ and $\epsilon_\downarrow(k) = -2\,t\,{\rm cos}k + U\langle n_\uparrow\rangle$.

(5) Finally, normalize your energy accumulator to the number of sites (divide by N) and add in the term $-U\langle n_\uparrow\rangle\langle n_\downarrow\rangle$. This gives the energy for the given $N_\uparrow$ and $N_\downarrow = N_{\rm tot} - N_\uparrow$. Make a list of them and see which is lowest.

(6) Repeat the calculation for different U and $N_{\rm tot}$ to get the phase diagram.

I will now show some real code for this problem and also a few results from running it.

A. The code

```
implicit none
integer i,N,Nup,Ndn,Ntot
real*8 t,U,tpin,k,ekup,ekdn,denup,dendn
real*8 efup,efdn,eftot

write (6,*) 'N,Ntot,t,U'
read  (5,*)  N,Ntot,t,U
tpin=8.d0*datan(1.d0)/dfloat(N)
do 1000 Nup=0,Ntot,2

Ndn=Ntot-Nup
denup=dfloat(Nup)/dfloat(N)
dendn=dfloat(Ndn)/dfloat(N)

efup=0.d0
efdn=0.d0
do 200 i=-N/2+1,N/2
    k=tpin*dfloat(i)
    if (i.ge.-Nup/2+1.and.i.le.Nup/2) then
       ekup=-2.d0*t*dcos(k)+U*dendn
       efup=efup+ekup
    endif
    if (i.ge.-Ndn/2+1.and.i.le.Ndn/2) then
       ekdn=-2.d0*t*dcos(k)+U*denup
       efdn=efdn+ekdn
    endif
200 continue
eftot=(efup+efdn)/dfloat(N)-U*denup*dendn

write (36,990) Nup,Ndn,eftot
990 format(2i6,f16.6)

1000 continue

end
```

B. Results for $\rho = \frac{1}{2}$

Here are results for one quarter filling, that is, a density $\rho = \rho_\uparrow + \rho_\downarrow = \frac{1}{2}$ electrons per site. (This is one quarter of the maximal density of two electrons per site.) The magnetization m is defined such that $m = (\rho_\uparrow - \rho_\downarrow)/(\rho_\uparrow + \rho_\downarrow)$.

You see that at $U/t = 2$ the optimal energy is paramagnetic: the energy E is minimized at $m = 0$. This is still the case at $U/t = 4$ (see next page), but the energy of the spin polarized solutions (m nonzero) are getting much closer to $m = 0$. (Note the energy scale.) When $U/t = 4.2$ the energies for large $|m|$ have started to turn down and are lower than

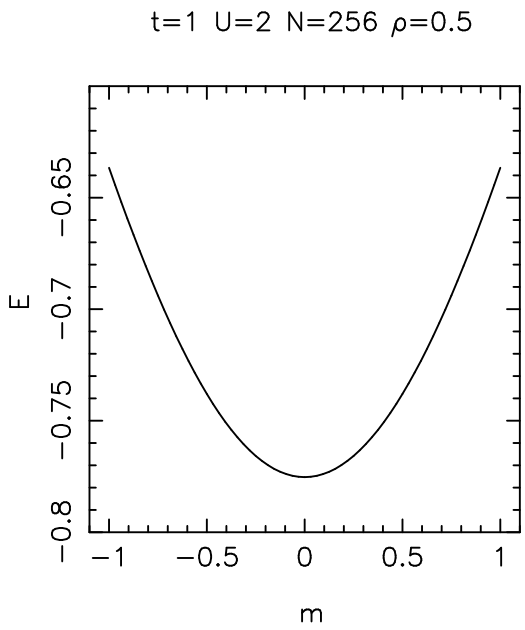


FIG. 1: Energy versus magnetization of $d = 1$ Hubbard model at $U/t = 2$ and $\rho = \frac{1}{2}$ (128 electrons on an $N = 256$ site lattice).

intermediate m, though $E(m = 0)$ is still lowest. $U/t = 4.4$ has just gone ferromagnetic.

Notice that the transition is *first order*. That is, as U/t increases we jump suddenly from a minimum at $m = 0$ to a minimum at $m = \pm 1$. Another possibility would have been a second order transition in which the minimum at $m = 0$ gradually shifts to larger m and partially polarized solutions are best for a range of U/t. Without examining other MF solutions (like antiferromagnetic ones) we cannot tell if this first order transition is 'real' or simply occurs because we have restricted to ferromagnetic solutions and something even lower in energy is actually winning.

C. Consistency with Stoner Criterion

We derived the Stoner Criterion for Ferromagnetism $UN(E_{\rm F}) > 1$. For the d=1 Hubbard model we can compute,

$$N(E) = 2\sum_k \delta(E - \epsilon_k) = 2\int \frac{dk}{2\pi}\delta(E - \epsilon_k)$$

with $\epsilon_k = -2t\cos(k)$. A simple calculation gives

$$N(E) = \frac{1}{\pi\sqrt{4t^2 - E^2}}. \tag{1}$$

(You also did this in Exercise 30.) This is the density of states for a single spin species, which is what was used in the Stoner criterion.

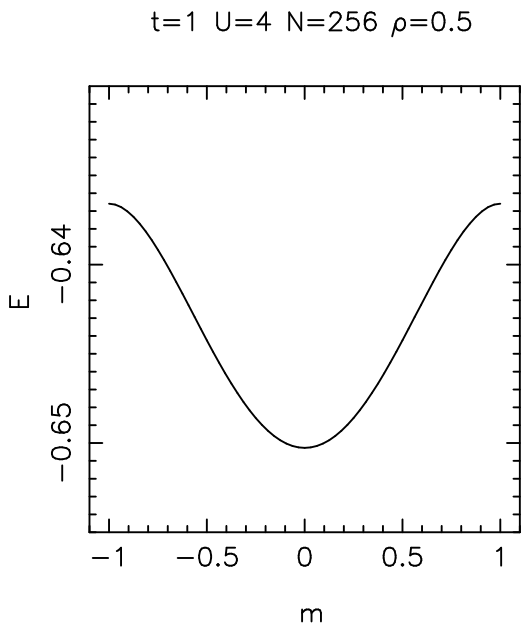


FIG. 2: Same as Fig. 1 except $U/t = 4$.

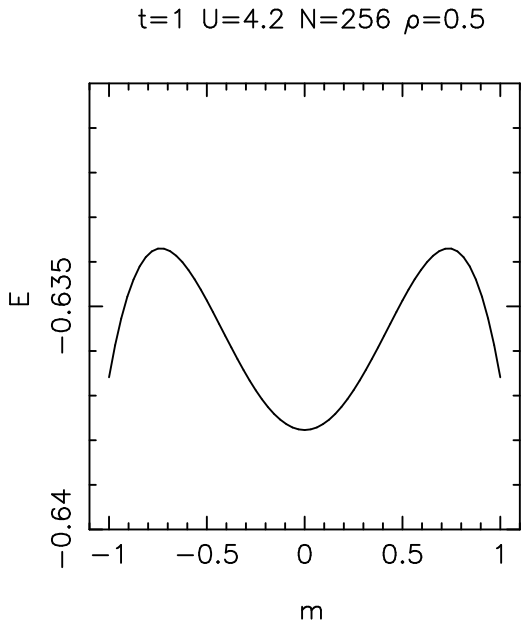


FIG. 3: Same as Fig. 1 except $U/t = 4.2$.

We also need the relation between the density ρ and the Fermi energy $E_{\rm F}$:

$$\rho = 2 \int_{-2t}^{E_{\rm F}} dE \; N(E). \tag{2}$$

I put in the factor of two for spin here, so that when I plug in ρ I use the total density

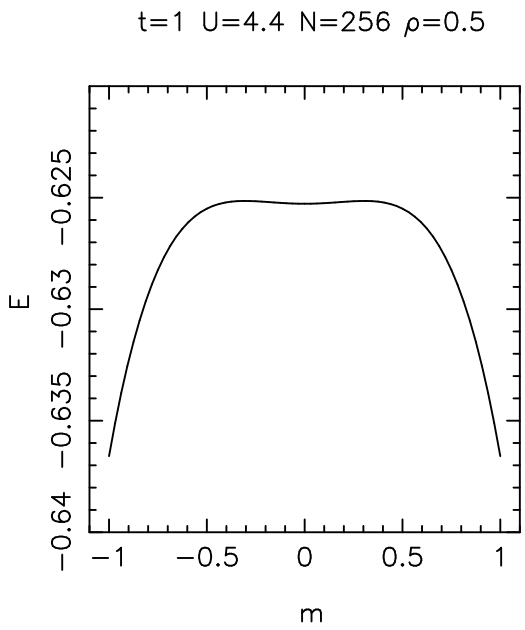


FIG. 4: Same as Fig. 1 except $U/t = 4.4$.

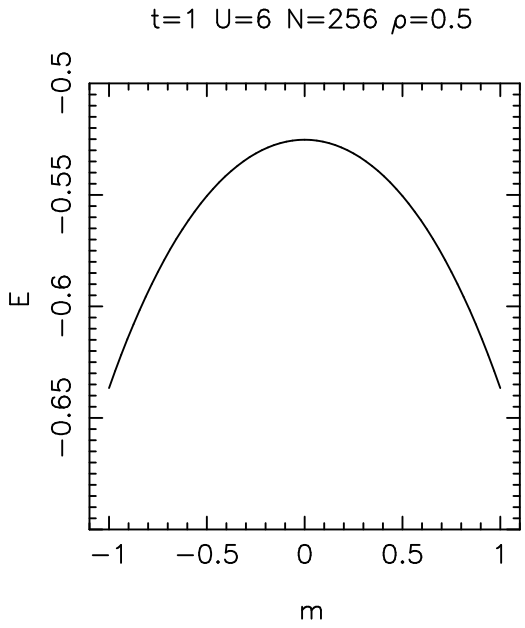


FIG. 5: Same as Fig. 1 except $U/t = 6$.

(including both spin species). This yields,

$$\rho = \frac{2}{\pi}\cos^{-1}(\frac{-E}{2t}). \tag{3}$$

You can check this latter relation obeys the expected limits: $\rho = 0$ when $E_{\rm F} = -2t$, $\rho = 1$ when $E_{\rm F} = 0$, and $\rho = 2$ when $E_{\rm F} = +2t$.

Putting these equations together, we can get the density of states at $E_{\rm F}$ for a given filling:

$$N(\rho) = \frac{1}{2\pi t}\frac{1}{\sin(\pi\rho/2)} \tag{4}$$

For half-filling, $\rho = 1$ we see that $N(\rho = 1) = \frac{1}{2\pi t}$ and hence $U_{\rm crit} = 2\pi t$. For quarter-filling, $\rho = \frac{1}{2}$ we see that $N(\rho = 1) = \frac{1}{\sqrt{2}\pi t}$ and hence $U_{\rm crit} = \sqrt{2}\pi t = 4.44t$. This is in pretty good agreement with Figures 1–5 which showed us that $U_{\rm crit}$ was around $4.4t$. I suspect that the slight disagreement (Figure 4 suggests $U_{\rm crit}$ a bit less than $4.4t$ while Stoner gives $U_{\rm crit}$ a bit more than $4.4t$) is due to the fact that Figures 1-5 were run on $N = 256$ site lattices. That is, I believe the small difference is likely a finite size effect.

Exercise 56: Write a code to do mean field theory for the $d = 1$ Hubbard model as described above. Compute the critical U above which the ferromagnetic state is lower in energy than the paramagnetic one for $N_{tot} = 3N/4$.

Exercise 57: Verify that the critical U you obtained for ferromagnetism precisely agrees with the Stoner criterion. You will need to use the value for the density of state obtained in Exercise 30.

There is another way to write the code, which you might find easier. Work in the grand-canonical ensemble. That is, provide a chemical potential μ and then *compute* $N_\downarrow$ and $N_\uparrow$ by filling those levels which are below μ. The density then comes out of the choice of μ, and, indeed, you will need to tune μ to get the density you desire. (This process is a bit annoying.)

One advantage of this method is that one can let the code find the lowest energy configuration, instead of searching through all the possible choices of magnetization. This is done in the usual way: Start at some densities $n_\uparrow, n_\downarrow$, compute $E(n_\uparrow, n_\downarrow)$, and then alter $n_\uparrow, n_\downarrow$, to reduce E (using your favorite gradient descent algorithm or whatever). Continue iterating until you reach the minimum.

Another reason this second, 'grand canonical', approach is more convenient is that it is easy to do things at finite temperature. One simply replaces the process where one accumulates the energies of all levels $\epsilon_\sigma(k) < \mu$ with accumulating $\epsilon_\sigma(k)$ times the Fermi function $1/[1 + e^{\beta(\epsilon_\sigma(k)-\mu)}]$. (Likewise, one puts this Fermi function in the computation of the density). Another reason the grand canonical approach is sometimes preferable is that it also generalizes better to states where the lowest energy is more complex, 'striped phases' etc, where the density of electrons is allowed to depend in a completely general way on the lattice site and spin species. In that situation, though, there is usually no longer an analytic form for the energy levels and one has to diagonalize a matrix to get them.

Exercise 58: Write your own code to do mean field theory for the $d = 1$ Hubbard model in the grand canonical ensemble as described above. Again compute the critical U above which the ferromagnetic state is lower in energy than the paramagnetic one for $N_{tot} = 3N/4$.

Before concluding with the discussion of mean field theory, it should be emphasized that this mean field approach, while very useful in yielding insight into the possible phases of the system, is a completely uncontrolled approximation. Mean field theory overestimates the tendency for ordered phases, and can (and does) predict magnetic order where none occurs. Even if a particular phase transition is correctly predicted by mean field theory, the details of the transition (critical temperature, critical exponents, etc) are usually incorrect.

XIV. MEAN FIELD THEORY: ANTIFERROMAGNETISM

The basic idea to look for antiferromagnetism in the Hubbard model within mean field theory is the same as for ferromagnetism. The thing that is just slightly more difficult is to figure out the energy levels.

First, let's define precisely what an antiferromagnetic configuration is. Recall that a paramagnetic configuration has the same exact density $n_{l\sigma} = n$ regardless of site l or spin σ, and that a ferromagnetic configuration allows the density to depend on σ but not l: $n_{l\uparrow} = n_\uparrow$, and $n_{l\downarrow} = n_\downarrow$ (see above).

An antiferromagnetic configuration allows a simple *spatial* dependence in which the densities alternate: $n_{l\uparrow} = n + (-1)^l m$, $n_{l\downarrow} = n - (-1)^l m$. That is, the even sites have a surplus of up spin electron density: $n_{\mathrm{even}\uparrow} = n + m$, $n_{\mathrm{even}\downarrow} = n - m$. The odd sites have a surplus of down spin electron density: $n_{\mathrm{odd}\uparrow} = n - m$, $n_{\mathrm{odd}\downarrow} = n + m$. Note that the total number of up and down electrons in the whole system is the same, nN, and that each site has the same density $2n$, once the densities of the individual spin species are summed. More generally one might have some sort of mixed ferromagnetic and antiferromagnetic configuration.

The form of the Hamiltonian in mean field theory is, $H = \sum_{j,l} c^\dagger_{j\sigma} M_\sigma(j,l) c_{l\sigma}$, where $M_\sigma(j,l)$ has $-t$ just above and below the main diagonal, with $M_\uparrow(l,l) = U(n - (-1)^l m)$, or $M_\downarrow(l,l) = U(n + (-1)^l m)$ along the diagonal. The eigenvalues for this sort of tridiagonal matrix when the diagonal is constant ($m = 0$). When m is nonzero, the eigenvectors of momentum k and $k + \pi$ are mixed (see below for further discussion) and the eigenvalues become: $E(k) = \pm\sqrt{(-2\,t\,\mathrm{cos}k)^2 + (Um)^2} + Un$. Here k is now defined in a 'reduced zone', $k = 2\pi/N\{-N/4 + 1, -N/4 + 2, \ldots, +N/4\}$, so that there are still N eigenvalues as there should be for this N dimensional matrix (two eigenvalues for each k, but only half as many k. The eigenvalues are the same for $\sigma =\uparrow$ and $\sigma =\uparrow$.) You might want to check that these eigenvalues reduce to the old ones when $m = 0$. Can you also check the eigenvalues make sense when $t = 0$? (Check that all the counting (degeneracies) are correct!)

The process for computing the energy of an antiferromagnetis configuration is the same as the steps (1–5) above, with the replacement of the ferromagnetic eigenvalues by the antiferromagnetic ones. Since we are assuming the total up and down densities over the whole lattice are identical, one no longer loops over different $N_\uparrow$. However, one does have to loop over different m. More precisely, one fixes $n = N_{\mathrm{tot}}/2$ and then tries $m = 1/N, 2/N \ldots,$.

One reason this problem is worth doing is because of its formal connections to so many other problems in solid state physics. The most obvious is the opening of a gap in an energy band by a periodic potential $V(G)$ with wavevector G (e.g. see Ashcroft and Mermin). In our problem we can think of the up spin electrons as moving in a periodic potential which has period π resulting from the oscillating down spin density (and vice-versa). A gap is opened at $k = \pm\pi/2$. There is also a connection to simple phonon problems where one makes the masses or spring constants vary: $m_1, m_2, m_1, m_2, \ldots$ or $k_1, k_2, k_1, k_2, \ldots$. Again, the single phonon dispersion curve for uniform masses and springs breaks into two branches, optic and acoustic. Some of you are presently doing this problem in Physics 240B. There are many other examples.

A. The Code

```
implicit none
integer i,N,Ntot,istag
real*8 t,U,tpin,k,ek,mstag
real*8 rho,Umstag,Urho
```

```
      real*8 eaf,eaftot,lambdaminus

      write (6,*) 'N,Ntot,t,U'
      read  (5,*)  N,Ntot,t,U
      write (36,*) Ntot/2+1

      tpin=8.d0*datan(1.d0)/dfloat(N)
      rho=dfloat(Ntot)/dfloat(N)
      Urho=U*rho/2.d0

      do 1000 istag=0,Ntot,2

      mstag=dfloat(istag)/dfloat(N)
      Umstag=U*mstag/2.d0

      eaftot=0.d0
      do 200 i=-Ntot/4+1,Ntot/4
          k=tpin*dfloat(i)
          ek = -2.d0*t*dcos(k)
          lambdaminus=-dsqrt(ek*ek+Umstag*Umstag)
          lambdaminus=lambdaminus+Urho
          eaftot=eaftot+lambdaminus
200    continue
       eaftot=2.d0*eaftot/dfloat(N)-U*(rho*rho-mstag*mstag)/4.d0

      write (36,990) istag,eaftot
990   format(i6,f16.6)

1000  continue

      end
```

B. Results for $n = \frac{1}{2}$

Here are results for one quarter filling, that is, a density $n = n_\uparrow + n_\downarrow = \frac{1}{2}$ electrons per site. (This is one quarter of the maximal density of two electrons per site.) The staggered magnetization m_s is defined such that the up and down spin densities are $n_\uparrow = n + (-1)^i m_s$ and $n_\downarrow = n - (-1)^i m_s$.

For $U = 2$ the paramagnetic solution m_s=0 has lowest energy. We know too from the preceding note that $m = 0$ is the lowest of the ferromagnetic energies. Notice as a check on the codes that one can compare with Figure 1 and see that $E(m_s = 0) = E(m = 0)$.

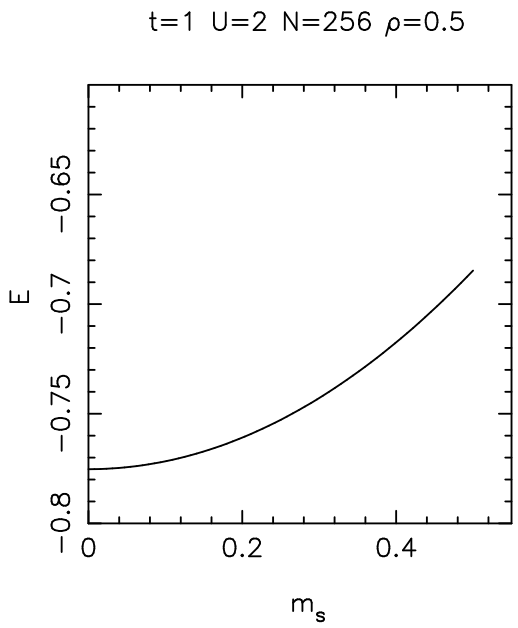


FIG. 6: Energy versus staggered magnetization of $d = 1$ Hubbard model at $U/t = 2$ and $\rho = \frac{1}{2}$ (128 electrons on an $N = 256$ site lattice).

As before, we now start cranking up U. Figures 2 and 3 show the energy for $U = 4$ and $U = 8$ respectively. We see at $U = 8$ that a nonzero m_s is better than zero m_s. However, the state is not actually antiferromagnetic because (Figure 4) the ferromagnetic energy is yet lower. (Again, check the fact that $E(m_s = 0) = E(m = 0)$. Really I should plot the ferromagnetic and antiferromagnetic data, Figures 3 and 4, on the same graph to make comparisons nicer.)

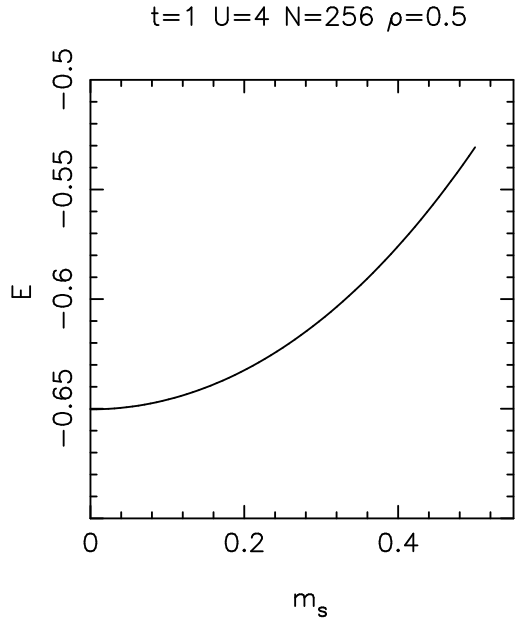


FIG. 7: Energy versus staggered magnetization of $d = 1$ Hubbard model at $U/t = 4$ and $\rho = \frac{1}{2}$ (128 electrons on an $N = 256$ site lattice).

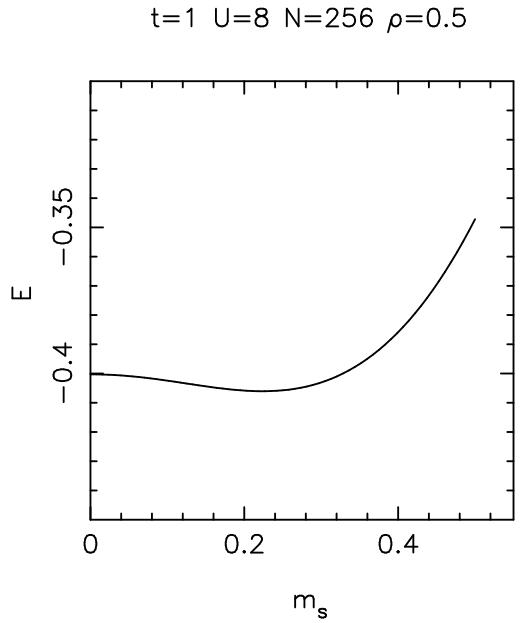


FIG. 8: Energy versus staggered magnetization of $d = 1$ Hubbard model at $U/t = 8$ and $\rho = \frac{1}{2}$ (128 electrons on an $N = 256$ site lattice).

C. Results for $n = 1$

The preceding results suggest that at quarter filling, $\rho = \frac{1}{2}$, the $d = 1$ Hubbard model is more prone to ferromagnetism than antiferromagnetism. Let's look at half-filling, $\rho = 1$, where antiferromagnetism tends to be most stable. Sure enough, Figures 5 and 6 show the

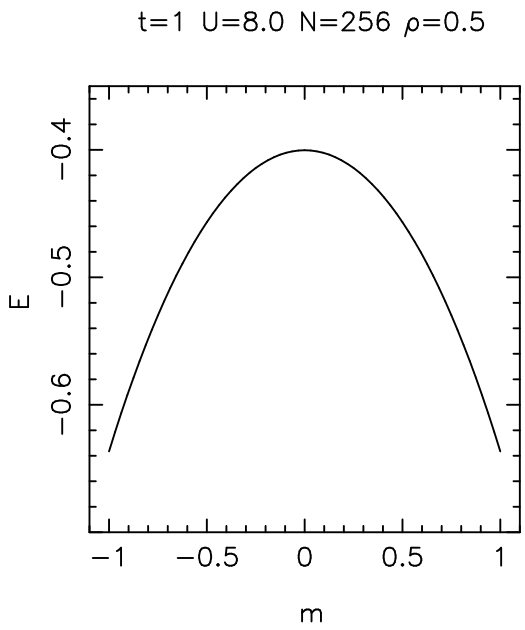


FIG. 9: Energy versus magnetization of $d = 1$ Hubbard model at $U/t = 8$ and $\rho = \frac{1}{2}$ (128 electrons on an $N = 256$ site lattice).

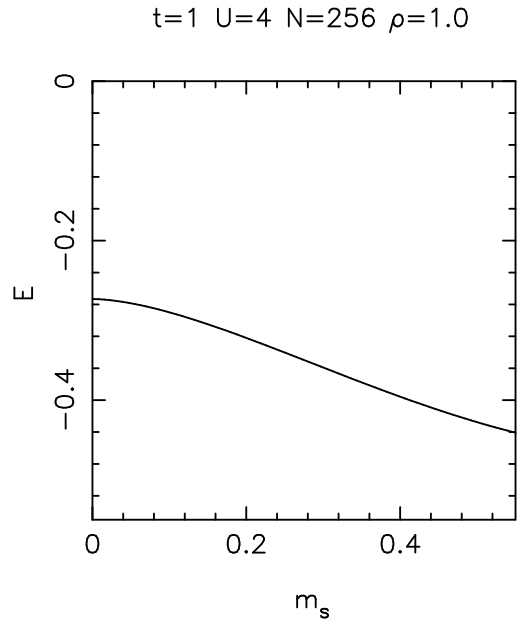


FIG. 10: Energy versus staggered magnetization of $d = 1$ Hubbard model at $U/t = 4$ and $\rho = 1$ (256 electrons on an $N = 256$ site lattice).

antiferromagnetism is optimal (for $U = 4$). In fact, here, the best m_s is the biggest it can be.

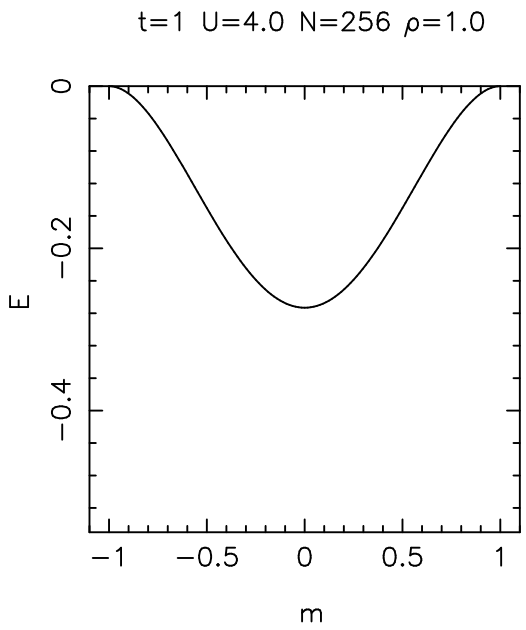


FIG. 11: Energy versus magnetization of $d = 1$ Hubbard model at $U/t = 4$ and $\rho = 1$ (256 electrons on an $N = 256$ site lattice).

D. Phase boundary

Our ultimate objective could be to analyze a bunch of energy curves, both ferro- and antiferromagnetic, for different densities ρ and couplings U and figure out the whole phase diagram in the $\rho - U$ plane. As a first step in this direction, Figure 7 shows the value of the staggered magnetization which minimizes the energy, as a function of density for different values of U. For small $U = 2$, the energy is minimized in the paramagnetic phase $m_s = 0$ until close to half filling ($\rho = 1$). As U increases, so does the regime of antiferromagnetism. For $U = 16$ the optimal staggered magnetization becomes nonzero around $\rho = 0.24$. So looking at the five points where m_s becomes nonzero begins to give us a sense of the antiferromagnetic phase boundary. We have to do similar analysis for the ferromagnetic case (and compare energies) to complete the picture.

XV. PARTICLE-HOLE SYMMETRY

The Hubbard Hamiltonian has a fascinating 'particle-hole' symmetry which allows us to relate its properties for different values of the parameters. Particle-Hole symmetry also plays an important role in quantum monte carlo simulations. Consider the introduction of new operators which exchange the role of creation and destruction:

$$d^\dagger_{\mathbf{i}\sigma} \quad = (-1)^{\mathbf{i}} c_{\mathbf{i}\sigma} \tag{5}$$

The meaning of the $(-1)^{\mathbf{i}}$ will be explained further below.

Exercise 59: Verify that the number operator for the d particles equals one minus the number operator for c particles: $d^\dagger_{\mathbf{i}\sigma} d_{\mathbf{i}\sigma} = 1 - c^\dagger_{\mathbf{i}\sigma} c_{\mathbf{i}\sigma}$. What happens to the interaction term in the Hubbard model $U(n_\uparrow - \frac{1}{2})(n_\downarrow - \frac{1}{2})$ under the particle-hole transformation?

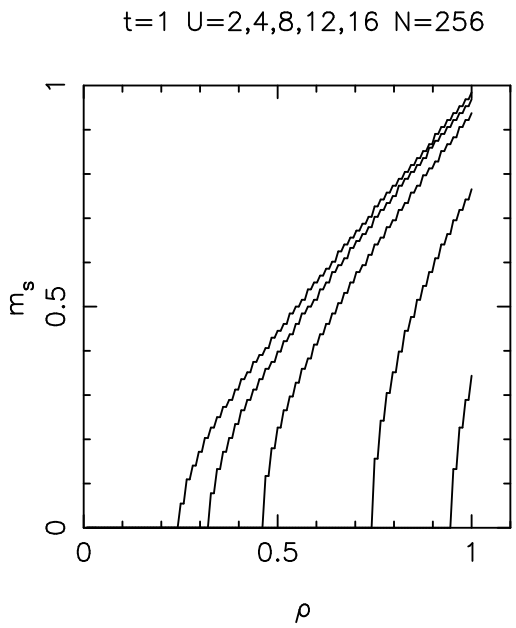


FIG. 12: Staggered magnetization m_s which minimizes the energy, as a function of density ρ for the $d = 1$ Hubbard model on a $N = 256$ site lattice. Curves are (left to right) $U = 16, 12, 8, 4, 2$.

Before seeing what happens to the kinetic energy term under a particle-hole transformation, we introduce the idea of a bipartite lattice. A bipartitie lattice is one which can be divided into two sublattices A and B in such a way that a site in A has neighbors which are all members of B and *vice-versa*. The $(-1)^{\mathbf{i}}$ factor in the particle-hole transformation takes the value -1 on one sublattice and $+1$ on the other.

Exercise 60: Is a one dimensional chain a bipartite lattice? How about a two-dimensional square lattice?

Exercise 61: Is the triangular lattice bipartite? What about the honeycomb lattice?

The following Exercise determines what happens to the kinetic energy term when the particle-hole transformation is performed.

Exercise 62: Verify that the kinetic energy is unchanged under a particle-hole transformation. That is, it takes exactly the same form in terms of the d operators as it did in terms of the c operators. Where does the bipartite nature of the lattice come enter? What role do the $(-1)^{\mathbf{i}}$ factors play?

What have we learned? Exercises 58 and 61 tell us that the Hubbard model, when the interaction term is written in the particle-hole symmetric form, is invariant under particle-hole transformations when $\mu = 0$. The condition $\mu = 0$ is necessary since the number operators which μ multiplies are not invariant but go into one minus themselves. Actually, a more precise statement is that the Hubbard model with a given μ maps into the Hubbard model with the sign of the chemical potential reversed, that is, with μ replaced by $-\mu$. In fact, this implies that the whole phase diagram of the Hubbard model on a bipartite lattice is symmetric about half-filling, as the following Exercises suggest.

Exercise 63: Show that the density of the Hubbard model on a bipartite lattice obeys the relation $\rho(\mu) = 2 - \rho(-\mu)$ by starting with $\rho = \langle n_\uparrow + n_\downarrow \rangle$ and making a particle-hole transformation.

Exercise 64: Show that the local moment of the Hubbard model on a bipartite lattice obeys the relation $\langle m^2 \rangle(\mu) = \langle m^2 \rangle(-\mu)$.

Exercise 65: Look back at you pictures of the density of states $N(E)$ obtained in Exercises 27-30 and explain their behavior when reflected about $E = 0$ in terms of particle-hole symmetry.

XVI. RELATION BETWEEN THE ATTRACTIVE AND REPULSIVE HUBBARD MODELS

It is also interesting to consider what happens when a particle-hole transformation is performed only on one of the spin species.

Exercise 66:

Show that if we perform the transformation,

$$\begin{aligned} d_{\mathbf{i}\uparrow} &= c_{\mathbf{i}\uparrow} \\ d_{\mathbf{i}\downarrow} &= (-1)^{\mathbf{i}} c^\dagger_{\mathbf{i}\downarrow} \end{aligned}$$

the sign of the interaction term reverses, while the kinetic energy remains unchanges.

The Hubbard model with $-U$ is called the attractive Hubbard model because a negative value of U represents an attraction between spin up and psin down electrons on the same site. By considering various operators one can show that magnetic order in the $+U$ Hubbard model is related to superconducting and charge order in the $-U$ Hubbard model, so that an understanding of the phases of one model immediately implies considerable information about the other.

Exercise 67: Show that under a particle-hole transformation of just the down spin species, the following operator mappings occur. (Ignore constants.)

$$\begin{aligned} m_{z,\mathbf{i}} = n_{\mathbf{i}\uparrow} - n_{\mathbf{i}\downarrow} \leftrightarrow n_{\mathbf{i}} = n_{\mathbf{i}\uparrow} + n_{\mathbf{i}\downarrow} \\ m_{+,\mathbf{i}} = c^\dagger_{\mathbf{i}\uparrow} c_{\mathbf{i}\downarrow} \leftrightarrow c^\dagger_{\mathbf{i}\uparrow} c^\dagger_{\mathbf{i}\downarrow} \\ m_{-,\mathbf{i}} = c^\dagger_{\mathbf{i}\downarrow} c_{\mathbf{i}\uparrow} \leftrightarrow c_{\mathbf{i}\downarrow} c_{\mathbf{i}\uparrow} \end{aligned}$$

The physical content of these results is that spin correlations along the z axis are interchanged with charge correlations, and spin correlations along the x and y axes (which are compinations of m_+ and m_-) are interchanged with pairing correlations.

XVII. WORLD MONTE CARLO IN ONE DIMENSION

A discussion of the path integral formulation of quantum mechanics, starting with the harmonic oscillator and then moving to quantum spins, bosons, and fermions, with an emphasis

on Quantum Monte Carlo, can be found at: http://leopard.ucdavis.edu/rts/resproj6.html by hitting the 'World-Line Quantum Monte Carlo" link (number 88).

A shorter discussion which starts immediately with the Heisenberg model can be found at: http://leopard.ucdavis.edu/rts/boulder.html by hitting the 'Lecture II (pdf file) link.

XVIII. DETERMINANT QUANTUM MONTE CARLO

A discussion of the determinant Quantum Monte Carlo method can be found at http://leopard.ucdavis.edu/rts/boulder.html by hitting the 'Lecture III (pdf file) link.

XIX. THE HUBBARD MODEL IN INFINITE DIMENSION- DYNAMICAL MEAN FIELD THEORY

One of the reasons for the continued interest in the Hubbard model is because of a recently developed approach known as 'dynamical mean field theory' (DMFT). This new technique has allowed for very interesting solutions of the Hubbard model itself, and also, more importantly, has provided a framework for the inclusion of Hubbard-type interactions into density functional theory. A 'popular' introduction to DMFT is available in: while a much more complete technical review is in: "Strongly Correlated Materials: Insights From Dynamical Mean-Field Theory," Physics Today, March, 2004. A. Georges, G. Kotliar, W. Krauth, and M. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).

XX. CONCLUSIONS

In these notes we have tried to provide an introduction to the Hubbard Hamiltonian and some of its elementary physics. We have seen how to write the model down and understand its behavior in the limit of no interactions, no kinetic energy, small clusters, and mean field theory. We have simply pointed to more sophisticated numerical methods and not mentioned at all the more complex analytic approaches, of which there are many indeed.

We have not mentioned at least one key piece of physics of the Hubbard model. the idea of a 'Kondo resonance'. It turns out that as one progresses from weak to strong coupling, the spectral function of the Hubbard model does not smoothly evolve from a single blob to two upper and lower Hubbard bands. Instead, sometime in the course of changing the interaction strength a three peak structure is in evidence: The beginning of the formation of upper and lower Hubbard bands, but also a sharp peak at the Fermi energy. Actually, it was originally thought that such peaks only arise in variants of the Hubbard model which contain both localized and delocalized electrons. It is only relatively recently that it was realized this sharp peak occurs in the Hubbard model as well. This very important idea is at the heart of much of the current research into the Hubbard model and its experimental realizations.