Electronic Hamiltonians - Part II

In the previous section we discussed electronic systems in the absence of electron-electron interactions, to understand the effects of the periodic potential on the eigenstates and eigenfunctions. Because we ignored electron-electron interactions, all we needed was to solve the problem for a single electron, to find the one-particle eigenstates and eigenfunctions. The many-body wavefunctions are then simply Slater determinants of such one-particle states, with the corresponding eigenenergies being the sum of the one-particle energies.

Clearly, the latter statement is not valid in systems with interactions, which is why such problems are very much more difficult to deal with. In fact, apart from a handful of very specific models (such as the Hubbard Hamiltonian in 1D), we do not know how to find exact many-electron eigenstates of interacting models. As a result, we are forced to use approximations. One of the most ubiquitous is the **Hartree-Fock approximation** (HFA). In the context of solid state systems, it is believed to be reasonably accurate if the e-e interactions are not too strong. Some of its predictions may also be ok for systems with strong e-e interactions (so-called **strongly correlated systems**), but there one has to be very careful to not fool oneself.

1 The Hartree-Fock Approximation

There are many different ways to justify this approximation. I will use the traditional variational approach and then I'll show you a different formulation, using a philosophy based on equations-of-motion that we'll also employ in a different context later on. But let me also say here that HFA can also be derived using diagrammatics (Green's functions and Feynman diagrams techniques, you will discuss these in Phys503). Roughly speaking, one can do perturbation theory in the e-e interaction, and the HFA turns out to be equivalent to keeping the first order corrections. It is for this reason that we are quite certain that HFA works well when the interactions are weak.

Let me also mention that most textbooks will suggest another method, that seems much simpler, namely, "factorization". The problem with that approach is that more often than not, it will give you the **wrong** answer, i.e. will produce a Slater dererminant that does not correspond to a global minimum of the total energy. This is because there is an infinite number of ways in which the Hamiltonian could be factorized, and the textbooks usually don't explain how to find the correct one. I will discuss in class more why that is so. In any event, don't be lazy when you do one of these calculations! Instead of using factorization, which might save a few minutes of work at the expense of almost certainly giving you the wrong results, it is better to use the variational approach (or even better, the faster equation-of-motion approach) which involve no guessing and are guaranteed to give you the lowest energy Slater determinant, i.e. the correct HFA solution.

1.1 The Ritz variational principle

Let $\hat{H}$ be a Hamitonian and let $E[\Psi] = \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle}$ be its average energy for any state $|\Psi\rangle$ from its Hilbert space. It then follows that any state $|\Psi\rangle$ for which this functional is stationary (i.e. $\delta E = 0$ for any small variations $|\delta\Psi\rangle$ about $|\Psi\rangle$) is an eigenstate of the Hamiltonian. You should be able to prove this last statement.

In practice, of course we cannot vary $|\Psi\rangle$ over the whole Hilbert space, in order to find the eigenstates, because that space is too big when we have many electrons in the system. The way we make use of this exact principle is to observe that $\forall|\Psi\rangle$, $E[\Psi] \geq E[\Psi_0] = E_0$, where $\hat{H}|\Psi_0\rangle = E_0|\Psi_0\rangle$

is the ground-state of the system. Again, you should be able to prove this statement (ask for help if you have trouble).

In practice, we restrict ourselves to a sector of the Hilbert space whose states $|\Psi\rangle$ are defined by a certain parameterization that allows us to "easily" calculate $E[\Psi]$. The particular $|\Psi\rangle$ that minimizes the energy is then used as an approximation for the true ground-state. How good this approximation is depends, of course, on how skilled we are in making a judicious choice for the form of the trial wavefunctions.

Note: I am talking about Hilbert spaces (as opposed to the full Fock space) because the way the HFA was introduced historically (way back when the 2ndQ notation had not yet been invented), it was convenient to assume a given, fixed number of electrons in the system. However, everything we do generalizes to open systems with varying numbers of electrons, as you'll see soon.

For the Hartree-Fock approximation, we restrict $|\Psi\rangle$ to be Slater determinants: so we look for the Slater determinant that has the lowest average energy, and we use it as an approximation for the ground-state. That's it! In other words, we're trying to see which non-interacting electron wavefunction (these are always Slater determinants) does best in describing the interacting system. You can now appreciate why for weak interactions, this choice is likely to work well – the system is not too far from where the ground-state is really a Slater determinant. For strongly interacting systems, however, there is no a priori reason to expect this to be a good choice. It sometimes works fairly well, for reasons that will become clearer as we work our way through this section, but it's never guaranteed to do so.

1.2 How the rest of this section is organized

There are two fairly disjoint goals we have for this section. One is for you to learn how to do HFA for model Hamiltonians, which are usually Hubbard-like models on various kinds of lattices with various kinds of interactions. This is needed because these are the types of models that you are likely to encounter in your research, and you ought to be able to deal with them.

The second goal is to study the HFA for the jellium model, and learn the physics that comes out of it. Of course, this problem has been solved long ago (although I'll argue that there are still parts that we don't understand well), so the focus here is primarily on the results. This is because the jellium model turns out to describe reasonably well what is known as "normal metals", and you must learn this phenomenology to (a) understand what normal metals are and how they behave, and (b) to appreciate how abnormal are the "strange metals" that don't behave normally (usually because they have strong correlations). In particular, this part will explain the screening and why, in certain materials, it is a good approximation that e-e interactions are weak.

Historically, the second part (jellium model) was done first, whereas the first is still on-going – you are likely to find HF results for some model Hamiltonian in any current issue of Physical Review B. As you may expect, the jellium model was dealt with using first quantization, because it was done before people came to appreciate how powerful the 2ndQ notation is (or, you could argue that doing these jellium model calculations in the 1stQ convinced people that maybe they should get better notation). For the jellium part, I will follow the traditional literature and use wavefunctions etc, partially because that is part of the common store of knowledge you should acquire, but also because it helps explain why we use certain language, eg calling HFA a "mean-field approximation". But I will also do my best to show that it is the same underlying method like the one we use to deal with model Hamiltonians (using 2ndQ), and hopefully once we're done with the first part, you will be able to figure the HFA for the jellium model on your own.

1.3 HFA for model tight-binding Hamiltonians

We start with an interacting Hamiltonian that is written in second quantization in terms of some known one-particle states, in the generic form:

$$\hat{H} = \sum_{\alpha,\beta} t_{\alpha,\beta} c_\alpha^\dagger c_\beta + \frac{1}{2} \sum_{\substack{\alpha\alpha' \\ \beta\beta'}} u_{\alpha\beta,\alpha'\beta'} c_\alpha^\dagger c_\beta^\dagger c_{\beta'} c_{\alpha'}$$

The first term collects all one-particle operators (kinetic energy and interaction with external fields, eg the ions), and the second one the e-e interactions. All the parameters $t_{\alpha\beta}, u_{\alpha\beta,\alpha'\beta'}$ are assumed to be known. For model Hamiltonians, α usually collects indexes specifying which orbital of which atom from which unit cell is in play (i.e., the electron is added or removed from that orbital), and as usual, what is its spin. In the following, I will call these "the old operators".

As I just said, in the HFA we're approximating the true ground-state with the "best" (meaning, the one of lowest total energy) Slater determinant. As we know only too well, Slater determinants are eigenfunctions of non-interacting Hamiltonians. So another way to think of HF is that we're trying to approximate the true Hamiltonian $\hat{H}$ by its "largest" diagonal part, i.e. we're trying to find the most accurate way to write it as:

$$\hat{H} \to \hat{\tilde{H}} = \sum_n E_n a_n^\dagger a_n$$

so that the (approximate) ground state is the Slater determinant $|HF\rangle = \prod_p a_p^\dagger |0\rangle$. For convenience, in this section I am using the convention that n, m label all the one-particle states; $p, p' = 1, ..., N$ labels the occupied states in the HF GS; and $h, h' = N+1, ...$ label the empty states in the HF GS. Thus, $\prod_p$ is shorthand for $\prod_{p=1}^N$ and involves only the occupied states.

Let's continue: so we have to find the "best" choice for the new one-particle states $|n\rangle$ associated with the operators a_n, and their energies E_n. Whatever this new basis is, it can be obtained through a unitary transformation from the old basis $|\alpha\rangle$ in which we wrote the Hamiltonian. Using $|n\rangle = a_n^\dagger |0\rangle = \sum_\alpha |\alpha\rangle\langle\alpha|n\rangle$ where $|\alpha\rangle = c_\alpha^\dagger |0\rangle$, we find:

$$a_n^\dagger = \sum_\alpha \langle\alpha|n\rangle c_\alpha^\dagger = \sum_\alpha u_n(\alpha) c_\alpha^\dagger \qquad\qquad a_n = \sum_\alpha \langle n|\alpha\rangle c_\alpha = \sum_\alpha u_n^*(\alpha) c_\alpha$$

Using the fact that the transformation is canonical, i.e. $\sum_n u_n^*(\alpha) u_n(\beta) = \sum_n \langle n|\alpha\rangle\langle\beta|n\rangle = \delta_{\alpha,\beta}$ and similarly $\sum_\alpha u_n^*(\alpha) u_m(\alpha) = \delta_{nm}$, we can also find the link between the old and the new operators:

$$c_\alpha^\dagger = \sum_n u_n^*(\alpha) a_n^\dagger \qquad\qquad c_\alpha = \sum_n u_n(\alpha) a_n$$

Now the stage is set. What we're trying to do is to find out how to pick these coefficients $u_n(\alpha)$ and the corresponding E_n such that $\langle HF|\hat{H}|HF\rangle / \langle HF|HF\rangle$ is minimized, i.e, the expectation value of the true Hamiltonian is as low as possible. In reality, to insure the normalization of the $|n\rangle$ states, and thus of $|HF\rangle$, it is more convenient that we add Lagrange multipliers for each of it and minimize $\langle HF|\hat{H}|HF\rangle - \sum_n E_n \langle n|n\rangle$ instead. Both procedures leads to the same result, so let me continue with the easier one with the Lagrange multipliers.

So what we have to do is to rewrite $\hat{H}$ in terms of the new operators (using the link between the old ones and the new ones given above), and then calculate its matrix element in the $|HF\rangle$

state using the fact that $a_n|HF\rangle = 0$ if $n > N$ (can't remove a particle that's not there to begin with), etc. The answer will depend on all the $u_n(\alpha), u_n^*(\alpha)$ coefficients, so we'll have some unappealingly long expression for $\langle HF|\hat{H}|HF\rangle = E(\{u_n(\alpha), u_n^*(\alpha)\})$. The second part is easy: $\sum_n E_n\langle n|n\rangle = \sum_{n,\alpha} E_n|u_n(\alpha)|^2$ - it also depends on these coefficients, of course. The optimal $u_n(\alpha)$ are obtained by requesting that the functional is minimized, i.e. that all its partial derivatives vanish, from which we obtain the so-called HF equations: $\frac{\partial E(\{u_n(\alpha),u_n^*(\alpha)\})}{\partial u_n^*(\alpha)} = E_n u_n(\alpha)$ for all $u_n(\alpha)$. Once we solve them, we have the optimal $u_n(\alpha)$ and the problem is done: we now know precisely what are the optimal new operators, and the corresponding $|HF\rangle$, and can calculate whatever other things we need to calculate.

While the steps to follow are straightforward, and we will actually practice soon how to calculate $\langle HF|\hat{H}|HF\rangle$ in terms of the $u_n(\alpha)$, I will not write all the intermediate formulae here because this is not the fastest way to get to the HF equations. So I will show you now another procedure that leads to the same HF equations, also without any guessing (unlike when using the factorization suggested in many textbooks) ... and does so faster and more easily. This is called the Equation-of-Motion (EoM) approach. There is a very nice book by D. J. Rowe called "Nuclear Collective Motion" that discusses its application to the HFA and other extensions like the RPA (don't worry about the title, nuclear physics also deals with strongly interacting many-body problems).

Consider how we would find the coefficients $u_n(\alpha)$ if the Hamiltonian was non-interacting, i.e. it could be put precisely in the form of $\hat{\tilde{H}}$. It is straightforward to check, using the usual anticommutation relations for fermionic operators, that:

$$[\hat{\tilde{H}}, a_n^\dagger] = E_n a_n^\dagger = E_n \sum_\alpha u_n(\alpha) c_\alpha^\dagger \rightarrow$$

$$E_n u_n(\alpha) = \{c_\alpha, [\hat{\tilde{H}}, a_n^\dagger]\} = \sum_\beta u_n(\beta)\{c_\alpha, [\hat{\tilde{H}}, c_\beta^\dagger]\}$$

If $\hat{\tilde{H}}$ is quadratic then $\{c_\alpha, [\hat{\tilde{H}}, c_\beta^\dagger]\}$ are just numbers, and the equations above give us eigenequations from which we can find $u_n(\alpha), E_n$.

The problem is that if we do this for our true Hamiltonian $\hat{H}$, because of its interaction terms we will find that $\{c_\alpha, [\hat{\tilde{H}}, c_\beta^\dagger]\}$ are operators, not numbers! So there is no way to have such an equality, between a number on the lhs ($E_n u_n(\alpha)$) and an operator on the rhs. What we do, then (and this turns out to be precisely equivalent to the variational HFA discussed before) is to ask that this equality holds in average, where the average is over the (as of yet unknown) HF GS:

$$E_n u_n(\alpha) = \sum_\beta u_n(\beta)\langle HF|\{c_\alpha, [\hat{H}, c_\beta^\dagger]\}|HF\rangle$$

These are the HF equations, identical to those coming from the minimization procedure discussed above. They are more easily obtained this way because we just have to calculate some commutators and anticommutators, which is fast with some practice (examples coming soon).

You should check at home (we might do parts of this calculation in class as practice, as well) that after doing those commutators, we find the HF equations to be:

$$E_n u_n(\alpha) = \sum_\beta t_{\alpha\beta} u_n(\beta) + \sum_{\alpha'} [U^H_{\alpha\alpha'} - U^E_{\alpha\alpha'}] u_n(\alpha') \tag{1}$$

where the Hartree and exchange terms are given by:

$$U^H_{\alpha\alpha'} = \sum_{\beta\beta'} u_{\alpha\beta,\alpha'\beta'} \sum_{p=1}^{N} u^*_p(\beta) u_p(\beta') \tag{2}$$

$$U^E_{\alpha\alpha'} = \sum_{\beta\beta'} u_{\beta\alpha,\alpha'\beta'} \sum_{p=1}^{N} u^*_p(\beta) u_p(\beta') \tag{3}$$

Notes: (i) to arrive at this final result, I used the fact that $u_{\alpha\eta,\beta\eta'} = u_{\eta\alpha,\eta'\beta}$, ie that both pairs of indexes can be interchanged. This comes directly from the meaning of $u_{\alpha\eta,\beta\eta'}$ as a two-particle matrix element, see Theorem 2 in the 2ndQ section. (ii) When we discuss the jellium model and its 1stQ approach, it will become clear why these terms are called "Hartree" and "Exchange".

The HF equations (1) are an eigenequation that we could solve to get the eigenenergies E_n and eigenvectors $u_n(\alpha)$, *if* the numbers $U^H_{\alpha\alpha'}, U^E_{\alpha\alpha'}$ were known. However, those numbers depend on the $u_n(\alpha)$, see Eqs. (2),(3), so we have a vicious circle: we need $U^H_{\alpha\alpha'}, U^E_{\alpha\alpha'}$ to get $E_n, u_n(\alpha)$, but we need to know $E_n, u_n(\alpha)$ to get $U^H_{\alpha\alpha'}, U^E_{\alpha\alpha'}$.

The way we deal with this is to solve the problem by iterations: we choose some values for $U^H_{\alpha\alpha'}, U^E_{\alpha\alpha'}$ (more on this below), and use them to solve the HF Eq. (1) and find the corresponding $E_n, u_n(\alpha)$. We then use these $E_n, u_n(\alpha)$ to calculate new values for $U^H_{\alpha\alpha'}, U^E_{\alpha\alpha'}$ from Eqs. (2),(3). If the old and the new values agree then the problem is solved. If not, then we start a new iteration where these newly obtained values of $U^H_{\alpha\alpha'}, U^E_{\alpha\alpha'}$ are plugged back into Eq. (1), etc etc. The iterations are repeated until we achieve **self-consistency**, i.e. the values that go into Eq. (1) agree with the values that come out of Eqs. (2),(3).

This might all sound a bit abstract and scary, but bear with me just a bit longer and you'll see that in practice things are much easier when we deal with a specific Hamiltonian, not with the most generic one that we can write, like here. Before going to examples, let me make a few more general comments, which will then be illustrated in specific examples.

1) as we'll see, there are always multiple self-consistent solutions for the HF equations. So how do we choose which is "the one"? The answer is easy: we take the best one, ie the one that minimizes the total energy. For any self-consistent set $E_n, u_n(\alpha)$, we can calculate the corresponding

$$E_{HF} = \langle HF|\hat{H}|HF\rangle = \sum_{\alpha,\beta} t_{\alpha,\beta} \langle HF|c^\dagger_\alpha c_\beta|HF\rangle + \frac{1}{2}\sum_{\substack{\alpha\alpha'\\ \beta\beta'}} u_{\alpha\beta,\alpha'\beta'} \langle HF|c^\dagger_\alpha c^\dagger_\beta c_{\beta'} c_{\alpha'}|HF\rangle$$

Using the link between old and new operators, we have:

$$\langle HF|c^\dagger_\alpha c_\beta|HF\rangle = \sum_{n,m} u^*_n(\alpha) u_m(\beta) \langle HF|a^\dagger_n a_m|HF\rangle$$

Remember that $|HF\rangle = \prod_p a^\dagger_p|0\rangle$. It follows that $\langle HF|a^\dagger_n a_m|HF\rangle = \delta_{n,m}$ if $n = m \leq N$ is an occupied state (in this case I can remove the particle and then add it back and return to the $|HF\rangle$ state I started with), and 0 otherwise. This is why:

$$\langle HF|c^\dagger_\alpha c_\beta|HF\rangle = \sum_p u^*_p(\alpha) u_p(\beta)$$

The second expectation value is calculated similarly. The key identity here is

$$\langle HF|a^\dagger_n a^\dagger_{n'} a_{m'} a_m|HF\rangle = \langle HF|a^\dagger_n a_m|HF\rangle\langle HF|a^\dagger_{n'} a_{m'}|HF\rangle - \langle HF|a^\dagger_n a_{m'}|HF\rangle\langle HF|a^\dagger_{n'} a_m|HF\rangle$$

in other words we can factorize the expectation value of the product of 4 operators into products of two-operator expectation values (which we already know how to calculate). This is only true if $|HF\rangle$ is a Slater determinant, and in fact it generalizes to a product of arbitrary many operators. The justification is that the one-particle states emptied when $a_{m'}$ and a_m act, must be filled back when $a_n^\dagger$ and $a_{n'}^\dagger$ act, otherwise the end state is different from $|HF\rangle$ and its overlap with $\langle HF|$ will vanish. So clearly either $n = m$ and $n' = m'$; or $n = m'$ and $n' = m$. In the later case, we inverted the order of removal and addition of fermions, hence the negative overall sign.

Putting everything together, we get:

$$E_{HF} = \sum_{\alpha,\beta} t_{\alpha,\beta} \sum_p u_p^*(\alpha) u_p(\beta)$$

$$+\frac{1}{2} \sum_{\substack{\alpha\alpha' \\ \beta\beta'}} u_{\alpha\beta,\alpha'\beta'} \left[\sum_p u_p^*(\alpha) u_p(\alpha') \sum_{p'} u_{p'}^*(\beta) u_{p'}(\beta') - \sum_p u_p^*(\alpha) u_p(\beta') \sum_{p'} u_{p'}^*(\beta) u_{p'}(\alpha') \right]$$

This looks a bit ugly (as I said before, when discussing the variational principle – imagine now starting to take derivatives from this beauty to get the HF equations. Clearly the EOM is easier.) but we do know all the numbers on the rhs, so we can find E_{HF}. We do this calculation for each self-consistent set, and the one with the lowest E_{HF} is declared as the HF solution.

2) How do we know that we've found all the self-consistent HF solutions? Because if we did not, we risk declaring a wrong one as the HF solution. The answer is that we're never truly sure, but to improve our chances we should do 2 types of searches. One is for "nice" states, for example we could try a homogeneous state (with equal number of electrons at each site) but also so-called charge-density-wave (CDW) states where the on-site number of electrons varies periodically in space, with more at one site and fewer at the next. Both are likely to give self-consistent solutions. We could also play with the spin, and search for paramagnetic states (zero average spin at any site), or ferromagnetic (FM) states (finite expectation for spin at all sites, all pointing the same way), or antiferromagnetic (AFM) states (alternating "up" and "down" spin expectation values). There are also more complicated spin orders, for example up, up, down, down repeated periodically, just like there can be more complicated electron density profiles that repeat periodically. We could also combine things, eg a CDW + AFM. So this is one way to generate searches – and as we'll see soon, once we decide what kind of state we're looking for, that gives us the $U^H_{\alpha\alpha'}, U^E_{\alpha\alpha'}$ to use in the first iteration.

But clearly, if we only do this, we may still miss the true HF state. So to be more sure, one should also do searches where $U^H_{\alpha\alpha'}, U^E_{\alpha\alpha'}$ are initiated as random numbers (this is called an **unrestricted** search, because we're not putting any input in the search), and we let the computer churn out to see what it finds. If it only find states like we've already tried (FM, or whatever) then after awhile we can stop the search and declare ourselves satisfied. However, if new self-consistent states are found, then we keep searching for more. Eventually nothing new will appear (or the new ones will have really high total energies, which makes them irrelevant) and we stop the search.

So we're never absolutely sure, but if we do this search well, we can be pretty confident that we found the Slater determinat of lowest energy, which we call the HF solution.

3) Let me go back to the energy $E_{HF} = \langle HF|\hat{H}|HF\rangle$, for which we got a rather ugly looking expression above. You might wonder why are we not using $E_{HF} = \sum_p E_p$, after all in this $|HF\rangle$ state we're occupying one-particle levels with energies E_p? The answer is that doing that is wrong, because $\sum_p E_p = \langle HF|\hat{\tilde{H}}|HF\rangle$. However $\hat{H} \neq \hat{\tilde{H}}$, so the two expectation values are NOT equal.

In fact, using the HFE we can re-arrange the correct expression that we found above to read:

$$E_{HF} = \langle HF|\hat{H}|HF\rangle = \sum_p E_p - \frac{1}{2}\sum_p \sum_{\alpha,\alpha'} u_p^*(\alpha)[U^H_{\alpha\alpha'} - U^E_{\alpha\alpha'}]u_p(\alpha')$$

The first term would be the answer if the particles were non-interacting. But they do interact, and one consequence of those interactions is the correction reflected in the second term (which, indeed, vanishes if the interactions vanish).

1.4 HFA for the Hubbard model

The results above are very general, as they hold for any Hamiltonian with any $t_{\alpha\beta}$ and $u_{\alpha\alpha',\beta\beta'}$ parameters. But because of this, it is a bit hard to get any clear feeling for what is happening, so don't feel too bad if you're a bit lost or confused. The other problem is that such general results are written "nicely" in terms of the Hartree and exchange potentials and other such cosmetic things that we pretty much never do in practice.

Let's make things more clear and see how we solve such problems, in reality, by looking at a specific model. I will consider the 1D Hubbard model here – if you understand its HFA solution, you should be able to generalize to any other model Hamiltonian.

So let's consider a chain with PBC and N sites, and for specificity I will assume that the number of electrons $N_e = N$. However, note that there could be more or fewer electrons in the system, the only restriction is that $0 \leq N_e \leq 2N$ but any value in between can be investigated. The HF solution will depend on which electron density N_e/N we're setting, so keep in mind that the specific results below are only true when $N_e/N = 1$, i.e. we have in average one electron per site. This is also known as the **half-filled** case. In homework problems I might ask you what happens for other electron concentrations, and/or in other dimensions.

As usual, we assume a single valence orbital at each site $i = 1, ..., N$ and let $c_{i\sigma}, c^\dagger_{i\sigma}$ remove/add electrons with spin σ in that orbital at site i. The Hubbard model, then, is:

$$\mathcal{H} = -t\sum_{i,\sigma}\left(c^\dagger_{i,\sigma}c_{i+1,\sigma} + h.c.\right) + U\sum_i c^\dagger_{i,\uparrow}c_{i\uparrow}c^\dagger_{i,\downarrow}c_{i\downarrow}$$

It does have the generic form with one- and two-particle terms, but now with very simple expressions for the hoppings and the interactions. This will make our calculations much easier.

We will do the algebra together in class, because it's good practice for you. Because of that, here I will only list the main results, so far as the calculations go.

Following the notes, we're trying to find new operators $a^\dagger_{n\sigma} = \sum_i \phi_{n\sigma}(i)c^\dagger_{i\sigma}$, etc. Note that (a) I'm *assuming* that the spin remains a good quantum number for the new basis, so I'm writting it explicitly, leaving n to represent whatever other quantum numbers we need. As discussed below, the assumption that the spin is a good quantum number is not the most general option, but it turns out to be correct at half-filling. So for simplicity, I will make it upfront. (ii) I will use the notation $\phi_{n\sigma}(i) = \langle i, \sigma|n, \sigma\rangle$ because this is the amplitude of probability to find an electron at site i when it is in the state (n, σ) (so obviously it has spin σ). If you prefer to call it $u_{n\sigma}(i)$ instead, like we did in the general case, by all means do so. You can use any notation you like so long as you clearly define it.

Following the notes, the HF equations are given by:

$$E_{n\sigma}\phi_{n\sigma}(i) = \sum_j \langle HF|\{c_{i\sigma}, [\mathcal{H}, c^\dagger_{j\sigma}]\}|HF\rangle\phi_{n\sigma}(j)$$

After doing the algebra, we find:

$$\{c_{i\sigma}, [\mathcal{H}, c^\dagger_{j\sigma}]\} = -t\left(\delta_{i,j-1} + \delta_{i,j+1}\right) + U\delta_{ij}c^\dagger_{i-\sigma}c_{i-\sigma}$$

where $-\sigma$ is the spin opposite to σ. As a result, the HF equations are:

$$E_{n\sigma}\phi_{n\sigma}(i) = -t\left[\phi_{n\sigma}(i-1) + \phi_{n\sigma}(i+1)\right] + U\langle HF|\hat{n}_{i,-\sigma}|HF\rangle\phi_{n\sigma}(i)$$

This has the generic form discussed before, but it only contains the "Hartree"part. For reasons that should become clear later on, when we discuss what the "exchange" part represents, that part vanishes for this model.

We also see the self-consistency appearing: to find the one-particle energies $E_{n\sigma}$ and the wavefunctions $\phi_{n\sigma}(i)$, we need to know the expectation values for $\langle HF|\hat{n}_{i,-\sigma}|HF\rangle$; but to calculate those, we need to know the wavefunctions first, as they define what is $|HF\rangle$. To be more specific, if we express the old operators in terms of the new ones, eg $c^\dagger_{i\sigma} = \sum_n \phi^*_{n\sigma}(i)a^\dagger_{n\sigma}$, we find:

$$\langle HF|\hat{n}_{i,-\sigma}|HF\rangle = \sum_m \phi^*_{m,-\sigma}(i)\sum_n \phi_{n,-\sigma}(i)\langle HF|a^\dagger_{m-\sigma}a_{n-\sigma}|HF\rangle = \sum_p |\phi_{p,-\sigma}(i)|^2$$

where the sum is over the occupied states with spin $-\sigma$. This should make good sense: the average number of electrons with spin $-\sigma$ found at site i is, indeed, the sum over all occupied states of the probability for finding a spin $-\sigma$ electron at the site i, when in that occupied state.

Now we're at the point where we should decide what type of state we're searching for, so that we have an initial guess for these $\langle HF|\hat{n}_{i,-\sigma}|HF\rangle$ (or use a computer to input random numbers and see what happens). As I said, beside the numerical search with random numbers, we can try various "simple" states for which we can solve the equations analytically.

Some of these simple states include:

(i) homogeneous and paramagetic. Homogeneity means that we have the same total charge at each site:

$$\langle HF|\hat{n}_{i,\uparrow}|HF\rangle + \langle HF|\hat{n}_{i,\downarrow}|HF\rangle = 1$$

(remember that we're dealing with the half-filled case. If the electron concentration was different, we'd have a different number on the rhs). Paramagnetic means zero expectation value for the spin at any site, in particular:

$$\langle HF|\hat{S}_{z,i}|HF\rangle = \frac{1}{2}\left[\langle HF|\hat{n}_{i,\uparrow}|HF\rangle - \langle HF|\hat{n}_{i,\downarrow}|HF\rangle\right] = 0.$$

From these two, it follows that such a state has $\langle HF|\hat{n}_{i,\uparrow}|HF\rangle = \langle HF|\hat{n}_{i,\downarrow}|HF\rangle = \frac{1}{2}$, and in this case the HF equation becomes:

$$E_{n\sigma}\phi_{n\sigma}(i) = -t\left[\phi_{n\sigma}(i-1) + \phi_{n\sigma}(i+1)\right] + \frac{U}{2}\phi_{n\sigma}(i)$$

We have to solve this problem, which hopefully you know how to do. Why? Because it is the same equation we would have for a non-interacting 1D chain with nearest-neighbor hopping and which has on-site energy $\frac{U}{2}$ at each site. We know that that system is invariant to lattice translations by a so the other quantum number must be the momentum k, restricted to the Brillouin zone $(-\frac{\pi}{a}, \frac{\pi}{a}]$. We also know that there is no other quantum number needed, because for N lattice sites there are $2N$ orbitals in the original basis set, therefore the N allowed k-values

in the BZ times the spin, account for all the states. So the wavefunctions are the usual Bloch states: $\phi_{n\sigma}(i) \to \phi_{k\sigma}(i) = \exp(ikR_i)/\sqrt{N}$ and $E_{k\sigma} = -2t\cos(ka) + \frac{U}{2}$. It then follows that the occupied states have $-\frac{\pi}{2a} \leq k \leq \frac{\pi}{2a}$ and it's straightforward to check that in this case, we indeed find $\langle HF|\hat{n}_{i,\uparrow}|HF\rangle = \langle HF|\hat{n}_{i,\downarrow}|HF\rangle = \frac{1}{2}$, so this solution is indeed self-consistent.

What is the total energy of this state? It's fastest to calculate it from scratch as opposed to trying to use previously derived formulae (which you might not have access to during an exam, and misremember). So here we go:

$$E^{(1)}_{HF} = -t\sum_{i,\sigma}\langle HF|c^\dagger_{i\sigma}c_{i+1,\sigma} + hc|HF\rangle + U\sum_i \langle HF|\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}|HF\rangle$$

Second part is always easier: if you factorize as we discussed before, here we find $\langle HF|\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}|HF\rangle = \langle HF|\hat{n}_{i\uparrow}|HF\rangle\langle HF|\hat{n}_{i\downarrow}|HF\rangle - \langle HF|c^\dagger_{i\uparrow}c_{i\downarrow}|HF\rangle\langle HF|c^\dagger_{i\downarrow}c_{i\uparrow}|HF\rangle = \frac{1}{4}$ (the expectation values in the second part vanish – if the spin is a good quantum number, like we assumed, there's no way to remove a spin-up and add instead a spin-down and still be in the same state).

The first part is not too bad, either. Going to the new operators, we find: $\langle HF|c^\dagger_{i\sigma}c_{i+1,\sigma}|HF\rangle = \sum_{-\frac{\pi}{2a}\leq k\leq\frac{\pi}{2a}} \frac{e^{-ika}}{N}$ (the sum is restricted to only the occupied states). This is independent of i, σ, thus $\sum_{i,\sigma} ... = 2N....$ and we find, altogether:

$$E^{(1)}_{HF} = 2\sum_{-\frac{\pi}{2a}\leq k\leq\frac{\pi}{2a}} \epsilon(k) + N\frac{U}{4}$$

where $\epsilon(k) = -2t\cos(ka)$ is the free electron dispersion. You can see that indeed we can put this in the second form given in the general notes:

$$E^{(1)}_{HF} = 2\sum_{-\frac{\pi}{2a}\leq k\leq\frac{\pi}{2a}} E_k - N\frac{U}{4}$$

so indeed we find the correction due to interactions (second term) to what would otherwise be the energy if these particles were non-interacting (first term). But again, in practice we wouldn't bother doing this, the first expression is perfectly good for calculating the value of $E^{(1)}_{HF}/N = -\frac{4t}{\pi} + \frac{U}{4}$.

(ii) we could try homogeneous and ferromagnetic, i.e.

$$\langle HF|\hat{n}_{i,\uparrow}|HF\rangle + \langle HF|\hat{n}_{i,\downarrow}|HF\rangle = 1$$

and

$$\langle HF|\hat{S}_{z,i}|HF\rangle = \frac{1}{2}\left[\langle HF|\hat{n}_{i,\uparrow}|HF\rangle - \langle HF|\hat{n}_{i,\downarrow}|HF\rangle\right] = S_z.$$

S_z is as of yet unknown, but don't let that bother you. This means that now we must use $\langle HF|\hat{n}_{i,\uparrow}|HF\rangle = \frac{1}{2} + S_z, \langle HF|\hat{n}_{i,\uparrow}|HF\rangle = \frac{1}{2} - S_z$ and solve the corresponding HF equations. The other quantum number is still $n \to k$ with the same Brillouin zone $(-\frac{\pi}{a}, \frac{\pi}{a}]$ (the problem has invariance to the usual translations, there is no difference between sites, all have the same spin and the same electron density). The difference is that now the energies will depend explicitly on σ, i.e. $E_{k\uparrow} \neq E_{k\downarrow}$. The "up" band is shifted below the "down" band, explaining why in the ground state there are more "up" electrons than "down" ones, and hence some overall total spin at each site. You should try finishing this at home, in particular find for what value of S_z is this solution self-consistent, and whether its energy is below or above that of $E^{(1)}_{HF}$ considered above.

(iii) a paramagnetic CDW, i.e.

$$\langle HF|\hat{n}_{i,\uparrow}|HF\rangle + \langle HF|\hat{n}_{i,\downarrow}|HF\rangle = 1 + (-1)^i\delta$$

and

$$\langle HF|\hat{S}_{z,i}|HF\rangle = \frac{1}{2}\left[\langle HF|\hat{n}_{i,\uparrow}|HF\rangle - \langle HF|\hat{n}_{i,\downarrow}|HF\rangle\right] = 0$$

The charge alternates between larger and smaller, but the total number of electrons in the system is still the correct N. Again, the value of δ is not known yet, it will come from the self-consistency.

Now we have $\langle HF|\hat{n}_{i,\uparrow}|HF\rangle = \langle HF|\hat{n}_{i,\downarrow}|HF\rangle = \frac{1}{2}\left[1 + (-1)^i\delta\right]$ so plug these guesses into the HF equations and solve. A bit of thinking should tell you that this problem is invariant only to $2a$ lattice translations, because even and odd sites are distinguishable by having different amounts of charge. So now k is in the smaller Brillouin zone $(-\frac{\pi}{2a}, \frac{\pi}{2a}]$, and we'll have two Bloch states we can form for each k, one for even sites and one for odd sites. We can then diagonalize the Hamiltonian to find which linear combinations are the true eigenstates, and what are their energies (because we have 2 bands in the Brillouin zone, you have to be careful which is filled and how much). Finally, once we have this information we can calculate the values for $\langle HF|\hat{n}_{i,\uparrow}|HF\rangle, \langle HF|\hat{n}_{i,\downarrow}|HF\rangle$ and ask that they be equal to $\frac{1}{2}\left[1 + (-1)^i\delta\right]$. This will give us the self-consistency equation that will only hold for a specific value of δ - so that fixes its value. Finally, we can again go on and calculate $E^{(3)}_{HF}$ for this state and compare it with the answers from the first 2 states, to see which is lower.

I am not giving the results for cases (ii) and (iii) here because it turns out that they are NOT the HF solution for this problem at half-filling, so while it's good practice for you to consider them, it is a bit of a waste of time for me to write down all those equations that turn out to be useless. The reason I mentioned these possibilities is that in other problems (some of which you may see in homeworks or exams), such FM or CDW states might be the correct HF state, so it's good to understand how to handle them. Also, when you solve a new problem, you don't know which is the HF so you should go through all these options. However, this specific problem has already been solved, and we know that the HF solution is, actually:

(iv) homogeneous and antiferromagnetic:

$$\langle HF|\hat{n}_{i,\uparrow}|HF\rangle + \langle HF|\hat{n}_{i,\downarrow}|HF\rangle = 1$$

and

$$\langle HF|\hat{S}_{i,z}|HF\rangle = \frac{1}{2}\left[\langle HF|\hat{n}_{i,\uparrow}|HF\rangle - \langle HF|\hat{n}_{i,\downarrow}|HF\rangle\right] = (-1)^i S$$

in other words the spin expectation values alternate (I set $\hbar = 1$ but if you want, you can carry it around). S is called the **staggered magnetization**. Combining the two we find:

$$\langle HF|\hat{n}_{i,\sigma}|HF\rangle = \frac{1}{2} + \sigma S(-1)^i$$

where S will be found self-consistently. Putting this into the HF equations leads to:

$$E_{n\sigma}\phi_{n\sigma}(i) = -t\left[\phi_{n\sigma}(i-1) + \phi_{n\sigma}(i+1)\right] + U\left(\frac{1}{2} - \sigma(-1)^i S\right)\phi_{n\sigma}(i)$$

To solve this, we realize that we have a two-site unit cell (even sites are distinct from odd sites because of different spin). So the unit cell has length $2a$ and there are $N/2$ over them, meaning the Brillouin zone is $-\frac{\pi}{2a} < k \leq \frac{\pi}{2a}$ and has $\frac{N}{2}$ equidistant allowed k values. So symmetries and

simple counting tell us that there will be two bands, thus $n \to k, \pm$ where k is the momentum and I'll use the second index $\pm$ to distinguish which band I'm talking about.

Next, we must decide what the wavefunctions $\phi_{n\sigma}(i) \to \phi_{k,\pm,i}(i)$ must look like. Symmetries tell us that these must be Bloch states. We know that we can form two Bloch states from our two orbitals per unit cell, one from the even sites, and one from the odd sites. The most general solution will be a linear combination of the two, so it must have the form:

$$\phi_{k,\pm,\sigma}(2i) = \alpha_{k,\pm,\sigma}\frac{e^{ikR_{2i}}}{\sqrt{N/2}}; \phi_{k,\pm,\sigma}(2i+1) = \beta_{k,\pm,\sigma}\frac{e^{ikR_{2i+1}}}{\sqrt{N/2}};$$

where normalization requires that $|\alpha_{k,\pm,\sigma}|^2 + |\beta_{k,\pm,\sigma}|^2 = 1$. Clearly, if $\alpha = 1$ and $\beta = 0$, we regain the Bloch state centered only on even sites, and viceversa. So we allow for any α, β (satisfying the normalization) in order to form the most general Bloch state possible.

Putting this guess in the HF equations, we find that:

$$\begin{cases} \left(E_{k,\pm,\sigma} - \frac{U}{2} + U\sigma S\right)\alpha_{k,\pm,\sigma} - \epsilon_k \beta_{k,\pm,\sigma} = 0 \\ -\epsilon_k \alpha_{k,\pm,\sigma} + \left(E_{k,\pm,\sigma} - \frac{U}{2} - U\sigma S\right)\beta_{k,\pm,\sigma} = 0 \end{cases}$$

where $\epsilon_k = -2t\cos(ka)$. This leads to two distinct bands:

$$E_{k,\pm,\sigma} = \frac{U}{2} \pm E_k = \frac{U}{2} \pm \sqrt{\epsilon_k^2 + (US)^2}$$

So indeed we found our two bands, as expected from symmetry considerations. These two bands are separated by a gap $2US$, and because we have only half the states filled, this means that this is an insulator with the $-$ band filled and the $+$ band empty. So this solution is already VERY different from (i), which predicted a metal!

But we still need to find the value of S. We can do this in multiple ways. One is to calculate $E_{HF}(S) = \langle HF|\mathcal{H}|HF\rangle$ and ask that $\frac{dE_{HF}}{dS} = 0$ (we're always looking for the lowest possible energy). Generally you need to calculate E_{HF} anyway, to compare it with that coming from other self-consistent solutions, so you may as well use it for finding the self-consistent S.

A faster (fully equivalent) way is to use its definition:

$$S = \frac{1}{2}\left[\langle HF|\hat{n}_{2i,\uparrow}|HF\rangle - \langle HF|\hat{n}_{2i,\downarrow}|HF\rangle\right] = \frac{1}{2}\sum_k \left[|\phi_{k-\uparrow}(2i)|^2 - |\phi_{k-\downarrow}(2i)|^2\right] = \frac{1}{N}\sum_k \left[|\alpha_{k-\uparrow}|^2 - |\alpha_{k-\downarrow}|^2\right]$$

This should be straightforward to get, we've discussed how to calculate these expectations values in the general case. In particular, here we have to go through all the occupied states (all k in the - band) and see what is the difference in probability that the electron will have spin up vs spin down. Hopefully this formula makes very good sense to you. (Always check that things make sense! If they don't, either the algebra is wrong, or you're not quite understanding the physics properly, so some work is needed before moving on).

We now need to find the amplitudes $\alpha_{k,-,\sigma}$ corresponding to the $E_{k,-,\sigma}$ band. Using either of the equations from the 2×2 system above plus the normalization, we find:

$$\alpha_{k,\pm,\sigma} = \sqrt{\frac{1}{2}\left(1 \mp \frac{\sigma US}{E_k}\right)}$$

which leads to the self-consistency condition:

$$S = \frac{1}{N}\sum_k \frac{US}{\sqrt{\epsilon_k^2 + (US)^2}} \to \frac{a}{2\pi}\int_{-\frac{\pi}{2a}}^{\frac{\pi}{2a}} dk \frac{US}{\sqrt{4t^2\cos^2(ka) + (US)^2}}.$$

This gives either $S = 0$ (already considered, it was option (i)), or whatever value of S satisfies:

$$1 = \frac{a}{2\pi} \int_{-\frac{\pi}{2a}}^{\frac{\pi}{2a}} dk \frac{U}{\sqrt{4t^2 \cos^2(ka) + (US)^2}}.$$

This equation can be solved numerically for any given values of U, t to find the corresponding S – this is the self-consistent value, which increases from 0 to 1/2 (maximum allowed value) as U/t increases from 0 to ∞. In particular, for large U/t we can use a Taylor expansion of the integrand to find:

$$S = \frac{1}{2}\left[1 - \frac{t^2}{(US)^2} + ...\right] = \frac{1}{2}\left[1 - \frac{4t^2}{U^2} + ...\right]$$

because to this order of accuracy, we can replace $S = 1/2$ on the right-hand side. So we see that in this limit the spins become (almost) fully polarized. What happens is that the probability to find spins-up will be nearly 1 at even sites and 0 at odd sites, and viceversa. So in the limit $U \gg 1$ we have one electron per site, with alternating spins – this is an AFM (Mott) insulator.

As always, the last step is to calculate the total energy of this state. We could borrow formulae from the notes, or we can do it from scratch. My recommendation is to always do the latter. Taking the expectation value and using the link between the c and a operators, we find:

$$E_{HF,AFM} = -t \sum_{k\sigma} \sum_i \left[\phi^*_{k,-,\sigma}(i)\phi_{k,-,\sigma}(i+1) + h.c.\right] + U \sum_i \langle HF|\hat{n}_{i,\uparrow}|HF\rangle\langle HF|\hat{n}_{i,\downarrow}|HF\rangle$$

(as discussed, the other terms such as $\langle HF|c^\dagger_{i,\uparrow}c_{i,\downarrow}|HF\rangle$ vanish if the spin is a good quantum number; also, only the $-$ band is occupied so we only see contributions from it). But the terms in the second sum are all equal to $\frac{1}{4} - S^2$ and so that sum is simply $NU\left(\frac{1}{4} - S^2\right)$. Using the known wavefunctions in the first term and doing all sorts of lovely algebra, we find in the end:

$$E_{HF,AFM} = \frac{NU}{4} - \sum_k \left[\sqrt{\epsilon_k^2 + (US)^2} + \frac{\epsilon_k^2}{\sqrt{\epsilon_k^2 + (US)^2}}\right]$$

after we also use the self-consistency condition written above (in other words, this expression is true only at self-consistency). I put it in this form because it is now straightforward to verify that for any value of $S \neq 0$, this is more negative than the value of the metallic state (which corresponds to $S = 0$):

$$E_{HF,1} = -2\sum_{k\sigma} \epsilon_k + \frac{NU}{4} > E_{HF,AFM}$$

Similarly, you could check that the self-consistent AFM HF solution is better than all the other ones you could try by hand and/or numerically.

So HF predicts that a half-filled 1D Hubbard model is an insulator with long-range AFM order for any $U > 0$. Interestingly, the 1D Hubbard model is one of very few models that can be solved exactly, using Bethe's ansatz – so for once, we can check how good HF is. It turns out that the exact GS is insulating at all $U > 0$, so this is something HF gets right. However, there is no long-range AFM order. The exact solution shows that $\langle \hat{S}_{z,i}\rangle = 0$ at each site, however there are strong, *short-range* AFM correlations. We'll discuss this in more detail when we discuss strong interactions, and we'll understand why long-range AFM is the best we can do with a single Slater determinant to "mimic" the true situation. This is why I said that care must be taken in how much of the HF predictions we believe, in the limit of strong correlations. For weak interactions it usually does well.

1.5 Hartree-Fock for the CM Theory of Everything

While we're practicing HF for model Hamiltonians in the homework (because, as I said, this is what you are most likely to need to be able to do), let's now go back in time and see how to do GF for the CM Theory of Everything, and then we'll specialize it to the jellium model. This will allow us to understand some of the nomenclature used, and to learn phenomenology associated with normal metals, which are rather well described by the jellium model.

Let $\hat{H} = \hat{T} + \hat{V}_{ext} + \hat{V}$ be the total Hamiltonian, where the first term is the kinetic energy of the electrons, the second term is their external interactions (with the lattice of ions, for our purposes) and the third is the e-e interactions. Because the ions are assumed to be locked in their equilibrium positions, their contribution to the total energy is a constant that has no bearing on what the electrons are doing, so I will ignore it here.

Let $\phi_n(\vec{r}) = \langle \vec{r}|a_n^\dagger|0\rangle = \langle \vec{r}|n\rangle$ be the set of orthonormal one-particle spinor-wavefunctions, and the associated creation and annihilation operators, from which we build the Slater determinant. As of yet, we do not know either what are the quantum numbers n, nor what are these wavefunctions – the goal is to find them so as to minimize the total energy. In any event, the Slater determinant will then be:

$$|HF\rangle = \prod_{p=1}^{N} a_p^\dagger|0\rangle \equiv \prod_p a_p^\dagger|0\rangle$$

i.e. the state we get by occupying the N lowest-lying of these one-particle states. Note: I will continue to use indexes n, m when referring to all single-particle states; p, p' when referring only to the occupied ones, so $1 \le p, p' \le N$, and h, h' when referring to empty states, so $h, h' > N$.

We can use this basis to write the Hamiltonian in the second quantization as:

$$\hat{H} = \sum_{n,n'} \langle n|\hat{T} + \hat{V}_{ext}|n'\rangle a_n^\dagger a_{n'} + \frac{1}{2} \sum_{\substack{n,n' \\ m,m'}} \langle nm|\hat{V}|n'm'\rangle a_n^\dagger a_m^\dagger a_{m'} a_{n'} \tag{4}$$

and therefore we can calculate its average value $\langle HF|\hat{H}|HF\rangle = E_1 + E_2$ as follows:

$$E_1 = \sum_{n,n'} \langle n|\hat{T}+\hat{V}_{ext}|n'\rangle \langle HF|a_n^\dagger a_{n'}|HF\rangle = \sum_p \langle p|\hat{T}+\hat{V}_{ext}|p\rangle = \sum_{p,\sigma} \int d\vec{r} \phi_p^*(\vec{r},\sigma) \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\vec{r})\right] \phi_p(\vec{r},\sigma).$$

The first equality uses the fact $n - n'$ must be an occupied state, else $\langle HF|a_n^\dagger a_{n'}|HF\rangle = 0$. For the second equality I assumed that the external potential doesn't depend on spin, which is usually the case; but if it does, we can generalize and the sum will be over two spin indexes.

Similarly,

$$E_2 = \frac{1}{2} \sum_{\substack{n,n' \\ m,m'}} \langle nm|\hat{V}|n'm'\rangle \langle HF|a_n^\dagger a_m^\dagger a_{m'} a_{n'}|HF\rangle = \frac{1}{2} \sum_{p,p'} \Big[\langle pp'|\hat{V}|pp'\rangle - \langle pp'|\hat{V}|p'p\rangle\Big]$$

where we use the factorization discussed before, to calculate the matrix element.

These two-particle matrix elements are also known, see 2ndQ Theorem 2. Again, assuming that the e-e interaction $V(\vec{r} - \vec{r}')$ does not depend on the spin of the electrons, we find:

$$E_2 = \frac{1}{2} \sum_{p,p'} \int d\vec{r} \sum_\sigma \int d\vec{r'} \sum_{\sigma'} \phi_p^*(\vec{r},\sigma)\phi_{p'}^*(\vec{r'},\sigma')V(\vec{r}-\vec{r'}) \Big[\phi_{p'}(\vec{r'},\sigma')\phi_p(\vec{r},\sigma) - \phi_p(\vec{r'},\sigma')\phi_{p'}(\vec{r},\sigma)\Big]$$

We now have to minimize $E = E_1 + E_2$ but also subject to the constraints that the wavefunctions $\phi_n(\vec{r}, \sigma)$ are normalized. This leads to requesting that $\frac{\delta F}{\delta \phi_p^*(\vec{r},\sigma)} = 0$ where

$$F = \langle HF|\hat{H}|HF\rangle - \sum_n E_n \int d\vec{r} \sum_\sigma \phi_n^*(\vec{r},\sigma)\phi_n(\vec{r},\sigma)$$

where E_n are Lagrange multipliers to enforce the normalization constraints. Taking these functional derivatives, we arrive at the **Hartree-Fock equations**:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\vec{r}) + V_H(\vec{r})\right]\phi_p(\vec{r},\sigma) - \sum_{\sigma'}\int d\vec{r'} V_E^{\sigma\sigma'}(\vec{r},\vec{r'})\phi_p(\vec{r'},\sigma') = E_p\phi_p(\vec{r},\sigma) \qquad (5)$$

where

$$V_H(\vec{r}) = \int d\vec{r'} V(\vec{r}-\vec{r'}) \sum_{p,\sigma} |\phi_p(\vec{r},\sigma)|^2 = \int d\vec{r'} V(\vec{r}-\vec{r'}) n(\vec{r'})$$

I hope you can see the similarities and the differences compared to what we did before. The main difference is that we got this Hamiltonian in the 1stQ, and we used the "new" (unknown) basis to write it in 2ndQ, so we can only do the variational minimization with it. By contrast, model Hamiltonians are always given in 2ndQ in terms of operators related to the orbitals kept in the problem ("old" operators). There we could do either the minimization, or use the EOM to get the HF equations.

$V_H(\vec{r})$ is called the **Hartree** potential, and equals the average potential created by all electrons at point $\vec{r}$. It turns out that if one assumed a simpler trial wavefunction: $\Psi(x_1, ..., x_N) = \phi_1(x_1)\phi_2(x_2)\cdots\phi_N(x_N)$ (where $x_i = \vec{r}_i, \sigma_i$), ie treat electrons as if they were distinguishable objects, then this is the only term one would get (check it!). Of course, the problem with this wavefunction is that it is not properly antisymmetrized as it should be for indistinguishable fermions, and therefore it does not enforce the Pauli principle.

The second term:

$$V_E^{\sigma\sigma'}(\vec{r},\vec{r'}) = V(\vec{r}-\vec{r'}) \sum_{p=1}^{N} \phi_p^*(\vec{r'},\sigma')\phi_p(\vec{r},\sigma).$$

is called the **exchange potential**, and appears precisely because we're enforcing the Pauli principle by using proper Slater determinants as trial wavefunctions.

IF the spin is also a good quantum number, in other words if $p = \tilde{p}, \sigma_p$, where $\tilde{p}$ includes all other quantum numbers, then $\phi_p(\vec{r},\sigma) = \delta_{\sigma,\sigma_p}\phi_{\tilde{p},\sigma_p}(\vec{r})$. In this case, the expressions above simplify to:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\vec{r}) + V_H(\vec{r})\right]\phi_{\tilde{p},\sigma_p}(\vec{r}) - \int d\vec{r'} V_E^{\sigma_p\sigma_p}(\vec{r},\vec{r'})\phi_{\tilde{p},\sigma_p}(\vec{r'}) = E_{\tilde{p},\sigma_p}\phi_{\tilde{p},\sigma_p}(\vec{r}) \qquad (6)$$

where $V_H = \int d\vec{r'} V(\vec{r}-\vec{r'}) n(\vec{r'})$ with $n(\vec{r'}) = \sum_{\tilde{p},\sigma_p} |\phi_{\tilde{p},\sigma_p}(\vec{r})|^2$ the total electron density like before, while:

$$V_E^{\sigma_p\sigma_p}(\vec{r},\vec{r'}) = V(\vec{r}-\vec{r'}) \sum_{\tilde{p}} \phi_{\tilde{p},\sigma_p}^*(\vec{r'})\phi_{\tilde{p},\sigma_p}(\vec{r})$$

has contributions only from electrons with the same spin σ_p! This should not be too surprising, because this term is due to the indistiguishability of electrons, as mentioned above. But only electrons with the same spin are indistinguishable (only such electrons can be in the same state, which is not allowed by Pauli; electrons with different spins are definitely not in the same state).

So that is why only same-spin electrons contribute this part, which comes from enforcing Pauli's principle. I'll return to this in a bit.

But first, let me mention that these HF equations also have the usual characteristic that we need to know V_H, V_E in order to find their eigenfunctions and energies, however V_H, V_E obviously depend on the (occupied) wavefunctions. So we'll need to find a self-consistent solution, either numerically by iterations, or by guessing the form of the wavefunctions up to some overall parameters, and then finding their values. And, of course, we again will find that there are multiple possible self-consistent solutions. The best is the one with the lowest total energy.

So what is the total energy of a self-consistent solution? You might be tempted to guess that it is $\sum_p E_p$, like it would be for non-interacting electrons, but never do that: interactions always change things! The good thing is that we've actually already calculated the answer: $E_{HF} = \langle HF|\hat{H}|HF\rangle = E_1 + E_2$ listed above. Adding those terms together (and assuming spin is a good quantum number, which will be the case in all the problems we study in this course), we find:

$$E_{HF} = \sum_{\tilde{p},\sigma_p} \int d\vec{r} \phi^*_{\tilde{p},\sigma_p}(\vec{r}) \left[\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\vec{r}) + \frac{1}{2}V_H(\vec{r}) \right) \phi_{\tilde{p},\sigma_p}(\vec{r}) - \frac{1}{2}\int d\vec{r'} V_E^{\sigma_p\sigma_p}(\vec{r},\vec{r'}) \phi_{\tilde{p},\sigma_p}(\vec{r'}) \right]$$

If it weren't for the factors of 1/2, the terms inside the square parentheses would match those on the lfs of the HF equation. So we can add and subtract what is needed to have that happen, and then use the HF equations and the orthonormalization of the eigenstates to find:

$$E_{HF} = \sum_{\tilde{p},\sigma_p} E_{\tilde{p},\sigma_p} - \frac{1}{2}\int d\vec{r} V_H(\vec{r}) n(\vec{r}) + \frac{1}{2}\int d\vec{r} \int d\vec{r'} \sum_{\tilde{p},\sigma_p} \phi^*_{\tilde{p},\sigma_p}(\vec{r}) V_E^{\sigma_p\sigma_p}(\vec{r},\vec{r'}) \phi_{\tilde{p},\sigma_p}(\vec{r'}) \quad (7)$$

Again, this shows that there is a correction, due to interaction, to the first term which represents the energy of non-interacting particles.

I hope you saw that even though the notation is quite different, the "guts" of the method and the structure of the HF equations, etc., are all very similar to what we did for model Hamiltonians.

2 HFA for the jellium model

Let us see how this works for the jellium model. We consider it because it is simple enough to solve analytically, so we won't need to make further approximations. This will allow us to learn many useful aspects of the physics, but of course there will be some wrong answers because the model is too simplified. Nevertheless, when used with proper care, this model offers a basic understanding of many properties of simple metallic systems.

In the following, I will assume that the true HF is homogeneous and paramagnetic. This turns out to be the correct answer for not too small electron densities, but not all (at very low electron densities, the correct HF is homogeneous but ferromagnetic, see homework).

For such a homogeneous state, and because we do not have a periodic potential, in other words because there is invariance to all translations, symmetry dictates that momentum is a good quantum number and therefore the HF one-particle states are characterized by $\vec{k}, \sigma$ and the HF eigenstates must be plane-waves $\phi_{\vec{k},\sigma}(\vec{r},\sigma') = \delta_{\sigma\sigma'} e^{i\vec{k}\vec{r}}/\sqrt{V}$. Like discussed previously, the allowed momenta $\vec{k}$ are dictated by the size of the box $V = L^3$, eg $k_x = \frac{2\pi}{L} m_x$, $m_x = 0, \pm 1, \pm 2, ...$ etc., but there is no restriction to a BZ because we have invariance to full translations, not to a discrete lattice group. So any momentum with components of this type is allowed, and in the limit $V \to \infty$ all momenta become allowed.

We assume that the corresponding energies $E_{\vec{k},\sigma}$ increase monotonically with increasing momentum. For a paramagnetic ground-state, i.e. one with equal number of spin-up and spin-down electrons, then

$$|HF\rangle = \prod_{\substack{|\vec{k}|<k_F \\ \sigma}} c^\dagger_{\vec{k},\sigma}|0\rangle$$

where the Fermi momentum k_F is defined such that precisely N states are occupied, i.e. $N = \sum_{\substack{|\vec{k}|<k_F \\ \sigma}} 1$. You should be able to show that in the limit $V \to \infty$, we have $k_F = (3\pi^2 n)^{\frac{1}{3}}$ where $n = N/V$ is the electron density.

Plugging all these into the HF equations we find immediately that:

$$E_{\vec{k},\sigma} = \epsilon(\vec{k}) - \frac{1}{V}\sum_{|\vec{k}|<k_F} u_{\vec{k}-\vec{k}'}$$

where $\epsilon(\vec{k}) = \frac{\hbar^2 k^2}{2m}$ is the kinetic energy of the free electrons. What happens here is that V_{ext} and V_H cancel out in Eq. (6), because the external potential is with the uniform density of ions, which is precisely counteracted by the V_H repulsion with the constant density of electrons. So we are left only with the exchange contribution, which is indeed negative and doesn't contain a sum over spins because only like-spins contribute to it. So it is exchange that lowers the energy from that of a free electron!

To make further progress, we need an expression for the e-e interaction. The most natural one is the Coulomb repulsion, in which case $u_{\vec{q}} = \frac{4\pi e^2}{q^2}$ (although it is by no means clear why this would be a "weak" interaction for which HF may work ok. I will return to this). Using the expression we have for the energy above, again in the thermodynamic limit where we can replace $\sum_{\vec{k}} f(\vec{k}) = \frac{V}{(2\pi)^3}\int d\vec{k} f(\vec{k})$, and after carrying out the integral, one finds:

$$E_{\vec{k},\sigma} = \epsilon(\vec{k}) - \frac{2e^2}{\pi}k_F F\left(\frac{k}{k_F}\right)$$

where the **Lindhard function** (in 3D) turns out to be:

$$F(x) = \frac{1}{2} + \frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right| \tag{8}$$

The next figures show (roughly) what this function looks like; what the corresponding energy $E_{\vec{k},\sigma}$ looks like, and what the corresponding density of states (DOS) looks like. Let me remind you that the DOS counts how many states (per unit volume) have a given energy E, i.e.

$$\rho(E) = \frac{1}{V}\sum_{\vec{k},\sigma}\delta(E - E_{\vec{k},\sigma}) \to \frac{1}{(2\pi)^3}\sum_\sigma \int d\vec{k}\delta(E - E_{\vec{k},\sigma}) = \frac{1}{\pi^2}\int_0^\infty dk k^2 \delta(E - E_k)$$

The first equality is the definition of DOS; the second holds in the limit $V \to \infty$, and the third holds if the energy depends only on the magnitude of the momentum and is independent of spin (like is the case in the expression above).

This result shows that because of interactions, the eigenenergy $E_{\vec{k},\sigma}$ is quite different from that of the free electron, $\epsilon(\vec{k})$. This is generically expected to be true. From now on I will call $E_{\vec{k},\sigma}$ the **quasiparticle** energy, because the actual object that is associated with it is not a free electron,

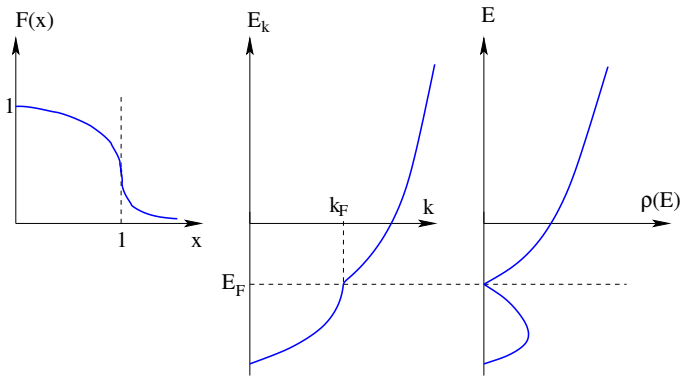

Figure 1: Left: Sketch of the Lindhard function $F(x)$, with its log singularity at $x = 1$; Middle: Sketch of the quasiparticle energy E_k, which inherits the log singularity at $k = k_F$ from the Lindhard function; Right: Sketch of the DOS, with a gap opening at E_F.

but instead is a composite of an electron and a cloud of particle-hole excitations that it creates because of interactions. We will return back to this in a bit.

In any event, quasiparticle energies are expected to be different from free-particle energies (and much of the challenge is to find out how). So this aspect of the solution is correct. What is wrong are some of the details. In particular, you can see that $F(x)$ has a log divergence in its slope at $k = k_F$, meaning that so does the quasiparticle energy, and that that happens precisely at the Fermi energy! Because of this log divergence, the DOS vanishes at the Fermi energy. This is totally wrong – for a metal we expect a robust (large) DOS at the Fermi energy, showing that there are available eigenstates to transport electrical currents and heat. So this **gap** that is predicted by our calculation is wrong, and going back we can figure out that it is there because we used $u_{\vec{q}} = \frac{4\pi e^2}{q^2}$, i.e. unscreened Coulomb interaction, as the interaction between electrons. If we had a form that did not diverge as $q \to 0$, these problems would be avoided. However, that would mean that the e-e interaction is not long-range, $1/r$-like, in other words that it is screened! As we will discuss soon, interactions are indeed screened, which is why in real metals we do not have a gap like that at the Fermi energy.

Let me also mention that such gaps at the Fermi energy (known as **Coulomb gaps**) can and do appear in **strongly disordered systems**, where the electronic states near the Fermi energy are strongly localized (definitely not plane-waves). But that is a very different situation from what we're discussing here – if we introduce a new ingredient (like strong disorder) we should expect that things can change dramatically. The bottom line is that in good clean metals there is a large DOS at the Fermi energy, and our model fails to describe this properly because of the unscreened form we used for the e-e interactions.

Before discussing in a bit more detail what is the quasiparticle and the screening issue, let us see if HFA predicts a stable system or not. For this we need to compute the total HF energy. According to the general formula, this turns out to be, after some simplifications:

$$E_{HF} = \sum_{\vec{k},\sigma} E_{\vec{k},\sigma} n_{\vec{k},\sigma} + \frac{1}{2V} \sum_{\substack{\vec{k}\neq\vec{k}' \\ \sigma}} u_{\vec{k}-\vec{k}'} n_{\vec{k},\sigma} n_{\vec{k}',\sigma}$$

where $n_{\vec{k},\alpha} = 1$ for an occupied state, i.e. if $|\vec{k}| < k_F$, and 0 otherwise. Note that $k_F = (3\pi^2 n)^{\frac{1}{3}}$ is

the same as for the free electrons, because it only counts how many states we have to fill to place all particles; their energy does not matter (ao long as it increases monotonically with k). This is a simple illustration of the so-called **Luttinger theorem**.

Using the expression for $E_{\vec{k},\sigma}n_{\vec{k},\sigma}$, we can further simplify this to:

$$E_{HF} = \sum_{\vec{k},\sigma} \epsilon(k) n_{\vec{k},\sigma} - \frac{1}{2V} \sum_{\substack{\vec{k}\neq\vec{k'} \\ \sigma}} u_{\vec{k}-\vec{k'}} n_{\vec{k},\sigma} n_{\vec{k'},\sigma}$$

where we can now easily identify the first term as being the contribution of the free electrons, and therefore the second must be due to interactions (remember, these include both the attractive interactions with the jellium positive background, and the repulsive interactions with all other electrons).

The first term is straightforward to calculate. It is customary to express the results in the following units: the energy unit is the Rydberg $1Ry = \frac{e^2}{2a_0} = 13.6eV$, where $a_0 = \frac{\hbar^2}{me^2} \approx 0.5\mathring{A}$ is the Bohr radius of a hydrogen atom. (These units should not be surprising because we are using a Coulomb potential for our interactions, so it's natural to compare to typical energies and legthscales for an electron trapped by its ion).

We can define a second lengthscale using

$$\frac{V}{N} = \frac{4\pi r_0^3}{3} \rightarrow r_0 = \left(\frac{3}{4\pi n}\right)^{\frac{1}{3}}$$

r_0 is thus the average distance between electrons because it defines the average volume available to each electron. This lenghtscale is related to k_F: $r_0 k_F \sim 2$ is a constant. In other words, the larger the density of electrons n, the smaller is the average distance r_0 between them, and the bigger is k_F needed to accommodate all of them. So we didn't really need to introduce r_0, we could have worked with k_F, but it is customary to do so and so we will.

Finally, we define:

$$r_s = \frac{r_0}{a_0}$$

as a dimensionless number that tells us how diluted or concentrated is the system. In regular metals, $r_s \approx 2 - 6$.

Using these units, you should verify that we can rewrite:

$$\frac{E_0}{N} = \frac{1}{N} \sum_{\vec{k},\sigma} \epsilon(k) n_{\vec{k},\sigma} = \frac{e^2}{2a_0} \frac{2.21}{r_s^2}$$

This is the contribution from the kinetic energy of the free electrons, and of course it is a positive number, meaning that if this was all the system would be unstable (the electrons would fly off in all directions). For an unscreened Coulomb potential we can calculate the second integral exactly (and you should do it once in your lifetime!) to find:

$$\frac{E_1}{N} = -\frac{1}{2V} \sum_{\substack{\vec{k}\neq\vec{k'} \\ \sigma}} \frac{4\pi e^2}{|\vec{k}-\vec{k'}|} n_{\vec{k},\sigma} n_{\vec{k'},\sigma} = -\frac{e^2}{2a_0} \frac{0.916}{r_s}$$

Thus, in Rydbergs, the HF energy per electron is:

$$\frac{E_{HF}}{N} = \frac{2.21}{r_s^2} - \frac{0.916}{r_s}$$

This is sketched below; it has a negative minimum (and thus, predicts a stable bound ground-state) for $r_s = 4.83$. Remember that in this model, all the contributions from interactions were due to the exchange term (the Hartree repulsion precisely cancels out the attraction from the jellium background). So the exchange term (which appeared because of enforcing the Pauli principle) is what provides the cohesion to keep the system stable.

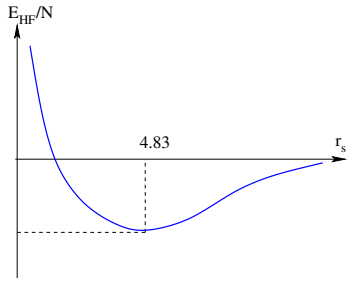

Figure 2: Sketch of E_{HF}/N vs r_s.

2.1 Pair correlations and the "Fermi hole"

To understand better what is happening, let us return to the HF equation (6) (where we assume that the spin is a good quantum number), and put it in a standard form $\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{tot}(\vec{r})\right)\phi_{\tilde{p},\sigma_p}(\vec{r}) = E_{\tilde{p},\sigma_p}\phi_{\tilde{p},\sigma_p}(\vec{r})$. This potential energy seen by the electron in state $\tilde{p},\sigma_p$ is then found to be:

$$V_{tot}(\vec{r}) = V_{ext}(\vec{r}) + V_H(\vec{r}) - \int d\vec{r'} V_E^{\sigma_p\sigma_p}(\vec{r},\vec{r'})\frac{\phi_{\tilde{p},\sigma_p}(\vec{r'})}{\phi_{\tilde{p},\sigma_p}(\vec{r})}$$

But

$$V_{ext}(\vec{r}) = -\int d\vec{r'} V(\vec{r}-\vec{r'}) n_{bk}(\vec{r'})$$

is the interaction with the positive background; for the jellium model, $n_{bk}(\vec{r'}) = n$ is a constant. The Hartree potential, as already discussed, is:

$$V_H(\vec{r}) = \int d\vec{r'} V(\vec{r}-\vec{r'}) n_H(\vec{r'})$$

where $n_H(\vec{r'})$ is the average electron density. Again, in the jellium model this is just n, which is why here these two terms precisely cancel each other out. Note, however, that if the positive ions were located on a lattice (as opposed to being uniformly spread throughout the space), the two densities would not necessarily be equal, because the average distribution of electrons in the unit cell would be more "spread around" than that of the positive ionic charge. So there would be a periodically modulated difference which would mean that the electron wavefunctions are Bloch states, not plane-waves, and solving for those makes this really complicated. Note also that I assumed that the electron-ion interaction is $-V(\vec{r}-\vec{r'})$ if the e-e interaction is $V(\vec{r}-\vec{r'})$; this is justified because no matter what this potential is (whether the full Coulomb or partially screened Coulomb or short-range or whatever), it should be modified in the same way – up to the different sign – for both types of electric charges.

Let's get back to our jellium model. Given all this, is it tempting to try to force the 3rd term to look like

$$\int d\vec{r'} V(\vec{r} - \vec{r'}) n_{ex}(\vec{r'})$$

so that we can see how the exchange term modifies the electronic density from the constant value predicted by the Hartree term (remember that Hartree corresponds to "distinguishable electrons", which don't obey the Pauli principle. The exchange term appeared because we implement the Pauli restriction for electrons with the same spin – as a result the wavefunction becomes a Slater determinant and we expect that this will change the electron density somehow from the Hartree prediction of a constant average. Now we're trying to see what this change is).

You can easily convince yourself that this form is not possible; the best we can do is to have it in a similar form but with a

$$n_{ex}^{\tilde{p},\sigma_p}(\vec{r},\vec{r'}) = \sum_{\tilde{q}} \phi^*_{\tilde{q},\sigma_p}(\vec{r'}) \phi_{\tilde{q},\sigma_p}(\vec{r}) \frac{\phi_{\tilde{p},\sigma_p}(\vec{r'})}{\phi_{\tilde{p},\sigma_p}(\vec{r})}$$

i.e. this density depends on which electron we consider (in which state) and where it is. We can define an average over all occupied states, to get a feeling for what this mean "exchange density" looks like in average:

$$n_{ex}(\vec{r},\vec{r'}) = \frac{2}{N} \sum_{|\vec{k}|<k_F} n_{ex}^{\vec{k},\sigma}(\vec{r},\vec{r'}) = 2n \left[\frac{1}{N} \sum_{|\vec{k}|<k_F} e^{i\vec{k}(\vec{r}-\vec{r'})} \right]^2$$

The second equality comes from putting plane-waves solutions for the our wavefunctions, i.e. it is only valid for the jellium model. The calculation is now straightforward (try it at home, come talk to me if you can't make it work) and we find, in terms of $\vec{\rho} = \vec{r'} - \vec{r}$, that:

$$n_{ex}(\rho) = \frac{9n}{2} \frac{[k_F\rho\cos(k_F\rho) - \sin(k_F\rho)]^2}{(k_F\rho)^6}$$

Note: we should feel good that this depends only on the distance $\vec{\rho} = \vec{r'} - \vec{r}$ because our system is invariant to full translations.

So, then, HF tells us that the average electron density that an electron that is at $\vec{r}$ sees at distance $\vec{r'} = \vec{r} + \vec{\rho}$, i.e. at relative distance $\vec{\rho}$ from where it is, is:

$$n_{HF}(\vec{\rho}) = n_H - n_{ex}(\vec{\rho}) = n \left[1 - \frac{9}{2} \frac{[k_F\rho\cos(k_F\rho) - \sin(k_F\rho)]^2}{(k_F\rho)^6} \right]$$

This is roughly sketched in the next figure. The average density is reduced to $n/2$ as $\rho \to 0$, showing that the electron repulses other electrons with the same spin (because of the Pauli principle), from its immediate neighborhood. The charge is thus rearranged and we can see some long-range oscillations because of this re-arrangement.

You can verify, by direct integration, that the "missing charge" is precisely equal to $+e$. This is known as **the Fermi hole**. It makes sense that it is $+e$ because one electron is at the origin and the remaining density must account for its absence from the rest of the system. We can now also understand the cohesion energy: think about the electron at the origin. At large distances, its attraction to the constant background is nearly perfectly cancelled by the repulsion with the

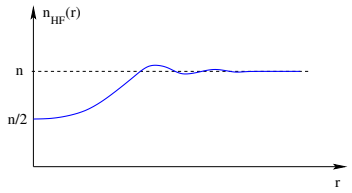

Figure 3: Average electron density at distance r from an electron, $n_{HF}(r)$ vs r.

(nearly constant) density of the other electrons. However, at short-range , because of the Fermi hole, there is more attraction to the positive background and this lowers the energy of this object compared to that of a free electron. In fact, now we can start to see an illustration of the idea of **quasiparticle**: the Pauli principle is responsible for the re-arrangement of the other electrons in the vicinity of an electron, in other words each electron always moves with this "bubble" of positive charge that surrounds it. So its motion must be such that everything else gets re-arranged accordingly, to make space for the bubble to move with the electron. This is why we use the word "quasiparticle" for the actual object that moves through the system.

However, we have to be VERY careful here with the language we use, and what is fact and what is approximation. Note that this bubble is there because we used a Slater determinant, which is a solution for non-interacting electrons. In other words, the wavefunction (and the bubble) is there even if there are no interactions between electrons, because the Pauli principle is always active. If there are no e-e interactions, then we talk about electrons (or particles), not quasiparticles. So you might wonder why with the same wavefunctions and the same hole, I talk about quasiparticles in the HF, versus particles if there is no e-e interaction.

Part of the reason is that the HF one-particle energies are modified from those of free electrons. So even though the "bubble" is the same at the HF level, the way the resulting object (the quasiparticle) moves is affected by interactions with all the other quasiparticles, which is why its energy is no longer $\epsilon(k)$ but $E_{\vec{k}}$. This is one difference. The better answer is to remember that HF is an approximation. In reality the true ground-state is not a Slater determinant, so the true bubble has a different distribution: the density is even lower at the origin, because the electrons with the other spin are also repulsed away from the origin when interactions are fully taken into account. So the "bubble" is different from that appearing for non-interacting electrons (i.e., the one due only to the Pauli principle), and then we can truly talk about a quasiparticle.

One way to further justify this, is to remind you that I stated that in a certain sense, HF can be thought of as the lowest order terms in a perturbative expansion in the strength of the e-e interactions. With MUCH effort, more terms in that expansion have been calculated, and now we know that for the jellium model in 3D

$$\frac{E_{GS}}{N} = \frac{e^2}{2a_0}\left[\frac{2.21}{r_s^2} - \frac{0.916}{r_s} + 0.0622\ln r_s - 0.096 + ...\right] = \frac{E_{HF}}{N} + \frac{E_{corr}}{N}$$

By definition, we call all terms not included in HF as **the correlation energy**, because they account for the effect of correlations in the wavefunction (Slater determinants are called non-correlated because they describe many-particle eigenstates in systems without interactions. Any other many-particle eigenstates have correlations, and they are stronger as the difference between the true wavefunction and a Slater determinant become bigger).

We are thus justified in talking about quasiparticles for interacting electrons because we know that the Slater determinant is an approximation, and in reality the wavefunction is more compli-

cated and it has a Fermi hole with a structure different from that of the non-interacting electron gas. The downside, of course, is that you should now wonder if we can even think in terms of HF quasiparticle states and energies, and what is their real physical meaning and usefulness. It turns out that in certain systems which are well described by the so-called **Fermi liquid theory**, this is a very useful notion. I will give you a few pointers about this at the end of this section, but first we need to discuss the screening issue a bit better.

3 Screening

Let me remind you that we concluded that it must be wrong to use the $1/r$ Coulomb potential (which is valid in vacuum) to describe the interactions between electrons and between electrons and ions in the solid, because this leads to the singularity at k_F which resulted in gap in the density of states, neither of which are observed in real materials. Neither would be there if we used a screened potential that decreases faster than $1/r$, so that it does not have the $1/q^2$ singularity in momentum space.

The notion of quasiparticle is useful to give us an intuitive idea about how screening occurs. If we think about the interactions between two quasiparticles, we have to remember that each electron is surrounded by its bubble of positive charge. Thus, if the two electrons are far enough from each other, they look like neutral objects to each other (repulsion with the other electron is cancelled by the attraction to its spherical bubble of positive charge). Another way to think about it is that all the other electrons (and positive charges, in a real system where we allow the ions to fluctuate about their equilibrium positions) re-arrange themselves so as to screen out internal fields and therefore the effective interactions between any two test charges (electrons and/or ions) vanish, if they are far apart. It is only when the two test charges are close to one another that this cannot happen, i.e. there aren't enough other charges in between that can re-arrange themselves to screen the fields out, and therefore the test charges will "feel" each other. This explains why we expect some short(er)-range interactions in solids, but the long range parts should definitely vanish much faster that $1/r$ (and so indeed, we do not have the gap in the DOS etc in real materials). Let us try to see how this works in a bit more detail, for the jellium model. Note that here only the other electrons are responsible for screening, because the positive background is not allowed to adjust its distribution to provide screening.

Let's start with some definitions. Suppose that we introduce some external charge in a system (the test charge – this could be one of our electrons, which we regard as being different from the rest of the system). If its density is $\rho_{ext}(\vec{r})$, the potential it would create in vacuum is given by the Poisson equation:

$$-\nabla^2\phi_{ext}(\vec{r}) = 4\pi\rho_{ext}(\vec{r}).$$

However, this test charge is not in vacuum, but in the solid that contains lots of mobile electrons. Because of the external potential created by the test charge, the electrons re-arrange themselves and this gives rise to an induced charge:

$$\rho_{ind}(\vec{r}) = -en(\vec{r}) + en$$

(the second term is the constant positive background. In the absence of the external charge and its potential, the electrons would be uniformly distributed and there would be zero induced charge). But now this induced charge also gives rise to a potential of its own. Let $\phi_{tot}(\vec{r})$ be the total potential due to the total charge:

$$-\nabla^2\phi_{tot}(\vec{r}) = 4\pi\left(\rho_{ext}(\vec{r}) + \rho_{ind}(\vec{r})\right).$$

Because we have a translationally invariant system, it is always better to work in momentum space, so let's Fourier transform all these quantities: $\rho_{ind}(\vec{r}) = \frac{1}{V}\sum_{\vec{q}} e^{i\vec{q}\vec{r}}\rho_{ind}(\vec{q})$ etc. Then, the two equations become:

$$q^2\phi_{ext}(\vec{q}) = 4\pi\rho_{ext}(\vec{q}) \qquad\qquad q^2\phi_{tot}(\vec{q}) = 4\pi\rho_{ext}(\vec{q}) + 4\pi\rho_{ind}(\vec{q})$$

from which we find:

$$\phi_{tot}(\vec{q}) = \phi_{ext}(\vec{q}) + \frac{4\pi}{q^2}\rho_{ind}(\vec{q})$$

i.e. the total potential is the external one plus that produced by the induced charge. So far so good, nothing too surprising. Now, we make the *assumption* that:

$$\rho_{ind}(\vec{q}) = \chi(\vec{q})\phi_{tot}(\vec{q})$$

where $\chi(\vec{q})$ is known as the **charge susceptibility**. This is known as a **linear approximation**, and it's valid in the limit when the total potential is small. If you think about solving the problem in perturbation theory, then the first correction is proportional to the applied "disturbance" and if this is small enough, we can ignore higher order, non-linear terms. For us this approximation is quite reasonable because remember that the other electrons will re-arrange themselves so as to screen out the external potential, in other words the total potential (that the electrons actually experience) should be quite small. So we'll stick with this approximation. Then, we find:

$$\phi_{tot}(\vec{q}) = \frac{\phi_{ext}(\vec{q})}{\epsilon(\vec{q})}$$

where

$$\epsilon(\vec{q}) = 1 - \frac{4\pi}{q^2}\chi(\vec{q})$$

is the dielectric function that you're already familiar with. For instance, if the test charge is an electron then $\rho_{ext}(\vec{r}) = -e\delta(\vec{r}) \to \phi_{ext}(\vec{q}) = -\frac{4\pi e}{q^2}$ is the usual Coulomb potential in vacuum, and the effective potential that this electron creates inside the solid is:

$$\phi_{tot}(\vec{q}) = -\frac{4\pi e}{\epsilon(\vec{q})q^2}$$

so it is indeed a screened or dressed potential. Note that here we assumed that we have no dynamics, but in reality these test charges may vary in time, in which case we have $\epsilon(\vec{q},\omega) = 1 - \frac{4\pi}{q^2}\chi(\vec{q},\omega)$, i.e. these functions depend on both momentum and frequency, generally. The static limit that we have been discussing corresponds to $\omega = 0$.

To understand the details of screening in the jellium model, we'll start with a very simple, semi-classical description first (which you might already know), and then we'll advance to a more accurate, QM calculation.

3.1 The Thomas-Fermi screening theory

This is valid if we assume that $\phi_{ext}(\vec{r})$ varies spatially very slowly, i.e. on a lengthscale much larger than the Fermi wavelength $\lambda_F \sim 1/k_F$. Tthen ρ_{ind} and ϕ_{tot} are also slowly varying, and the electrons experience a potential that is basically constant locally, and we can use the equations for

the homogeneous case. More specifically, we make the Thomas-Fermi (TF) approximation that the quasiparticle energies are:

$$E_k(\vec{r}) = E_k - e\phi_{tot}(\vec{r})$$

i.e. the total potential just shifts the quasiparticle energy by whatever value it has at that point. Then, the electron density is:

$$n(\vec{r}) = \frac{1}{V}\sum_{\vec{k},\sigma} \frac{1}{e^{\beta(E_k(\vec{r})-\mu)}+1} = n(\mu + e\phi_{tot}(\vec{r}))$$

where $n(\mu)$ is the dependence of electron density on the chemical potential, for the homogeneous system. So the potential simply shifts the chemical potential, such that more electrons will go where the potential is more attractive. The induced density, then, is:

$$\rho_{ind}(\vec{r}) = -en(\vec{r}) + en = -e\left[n(\mu + e\phi_{tot}(\vec{r})) - n(\mu)\right] \approx -e^2\phi_{tot}(\vec{r})\frac{\partial n}{\partial \mu}$$

Here, the last step is the linear approximation I already mentioned; indeed, if we Fourier transform we obtain:

$$\rho_{ind}(\vec{q}) = \chi(\vec{q})\phi_{tot}(\vec{q})$$

where $\chi_{TF} = -e^2\frac{\partial n}{\partial \mu}$ is a constant independent of q. The partial derivative is easy to calculate at $T = 0$, where $\mu = E_F = \hbar^2 k_F^2/2m$ and $k_F = (3\pi^2 n)^{\frac{1}{3}}$. Putting everything together, we find:

$$\epsilon_{TF}(q) = 1 + \frac{k_{TF}^2}{q^2}$$

where $k_{TF} = \sqrt{\frac{4k_F}{\pi a_0}}$ (a_0 is the Bohr radius) is a momentum that increases as the electron density n and thus k_F increase. The resulting screened potential created by a point charge is then:

$$V_{TF}(q) = \frac{4\pi e^2}{q^2 + k_{TF}^2} \rightarrow V_{TF}(r) = \frac{e^2}{r}e^{-k_{TF}r}$$

so the interaction now decreases exponentially, on a lenghtscale that decreases as n increases. This is a nice simple illustration of screening and how it modifies interactions from the $1/r$ of free vacuum. But of course, this is a bit too simple minded, so let's do a more accurate treatment to see how that is done and what it predicts.

3.2 Linear response theory

This is a general framework to discuss the response functions of a system (eg. the dielectric function we're interested in, but I'll mention a couple more examples below) to a small applied external field.

Let $\hat{H}_0$ and $|\Psi_0\rangle$ be the Hamiltonian for the unperturbed system, and its ground-state wavefunction, assumed to be known. If we apply a small external potential, then the Hamiltonian changes to:

$$\hat{H}(t) = \hat{H}_0 + \hat{H}_{ext}(t)$$

where the coupling to the external potential $\phi_{ext}(\vec{r}, t)$ is, in second quantization,

$$\hat{H}_{ext}(t) = -e\int d\vec{r}\hat{n}(\vec{r})\phi_{ext}(\vec{r}, t)$$

where $\hat{n}(\vec{r})$ is the electron density operator. This follows directly from the 1st quantization version of the interaction between electrons and an external potential, all we have to do is to write $\hat{n}(\vec{r})$ in 2nd quatization in whatever basis we want to use.

The challenge is to find $|\Psi(t)\rangle$ (assuming that at $t = -\infty$ the system was unperturbed, in its ground-state $|\Psi_0\rangle$), from which we can calculate the induced charge as the difference between its actual value and the unperturbed value:

$$\rho_{ind}(\vec{r},t) = -e\langle\Psi(t)|\hat{n}(\vec{r})|\Psi(t)\rangle + e\langle\Psi_0|\hat{n}(\vec{r})|\Psi_0\rangle$$

To find $|\Psi(t)\rangle$ we should solve the Schrödinger equation. It is convenient to work in the **interaction picture** where we define:

$$|\Psi_I(t)\rangle = e^{\frac{i}{\hbar}\hat{H}_0 t}|\Psi(t)\rangle$$

It is now straightforward to check that its equation of motion is:

$$i\hbar\frac{\partial|\Psi_I(t)\rangle}{\partial t} = \hat{H}_{ext,I}(t)|\Psi_I(t)\rangle$$

where

$$\hat{H}_{ext,I}(t) = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{H}_{ext}(t)e^{-\frac{i}{\hbar}\hat{H}_0 t}$$

is the coupling Hamiltonian in the interaction picture (I will use the subscript I for states and operators in this representation). Let me introduce the **evolution operator** $\hat{U}_I(t,t_0)$ defined such that $|\Psi_I(t)\rangle = \hat{U}_I(t,t_0)|\Psi_I(t_0)\rangle$ for any t, t_0; then the above equation translates into:

$$i\hbar\frac{\partial\hat{U}_I(t,t_0)}{\partial t} = \hat{H}_{ext,I}(t)\hat{U}_I(t,t_0) \rightarrow \hat{U}_I(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} d\tau\hat{H}_{ext,I}(\tau)\hat{U}_I(\tau,t_0),$$

which can be solved by iterations to find:

$$\hat{U}_I(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} d\tau\hat{H}_{ext,I}(\tau) + ...$$

where the ignored terms contain products of $\hat{H}_{ext,I}(\tau)$ operators and thus of external potentials (this is our linear approximation).

So we're now basically done, because $|\Psi_I(t)\rangle = \hat{U}_I(t,-\infty)|\Psi_0\rangle$. Using this plus the linear solution for $\hat{U}_I(t,t_0)$ and the fact that in the interaction picture we can rewrite:

$$\rho_{ind}(\vec{r},t) = -e\langle\Psi_I(t)|\hat{n}_I(\vec{r},t)|\Psi_I(t)\rangle + e\langle\Psi_0|\hat{n}(\vec{r})|\Psi_0\rangle$$

where $\hat{n}_I(\vec{r},t) = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{n}(\vec{r})e^{-\frac{i}{\hbar}\hat{H}_0 t}$, we finally get (again, to linear approximation) that:

$$\rho_{ind}(\vec{r},t) = \frac{ie}{\hbar}\int_{-\infty}^{t} d\tau\langle\Psi_0|[\hat{n}_I(\vec{r},t),\hat{H}_{ext,I}(\tau)]|\Psi_0\rangle = -\frac{ie^2}{\hbar}\int_{-\infty}^{t} d\tau\int d\vec{r'}\phi_{ext}(\vec{r'},\tau)\langle\Psi_0|[\hat{n}_I(\vec{r},t),\hat{n}_I(\vec{r'},\tau)]|\Psi_0\rangle$$

Let us define:

$$\Pi(\vec{r},t;\vec{r'},t') = -\frac{i}{\hbar}\theta(t-t')\langle\Psi_0|[\hat{n}_I(\vec{r},t),\hat{n}_I(\vec{r'},t')]|\Psi_0\rangle$$

with $\theta(x)$ being the Heaviside or step function. (This quantity is called a retarded Green's function, by the way; you'll learn all about them in Phys503). In terms of this, we have:

$$\rho_{ind}(\vec{r},t) = e^2\int_{-\infty}^{\infty} dt'\int d\vec{r'}\Pi(\vec{r},t;\vec{r'},t')\phi_{ext}(\vec{r'},t')$$

showing that $\Pi(\vec{r},t;\vec{r'},t')$ encodes the response of the system to any external potential, and can be calculated if we know the Hamiltonian and its ground state wavefunction. Note that the Heaviside function in the definition of $\Pi(\vec{r},t;\vec{r'},t')$ is essential to enforce causality in the equation above. It makes the integral stop at t (not infinity), showing that the induced charge only depends on the fields applied or times $t' < t$, as causality requires. We prefer to extend the integral to infinity (and add the Heaviside function) because that simplifies the Fourier transforms.

If the system is homogeneous and if $\hat{H}_0$ is independent of time, then it can be verified that $\Pi(\vec{r},t;\vec{r'},t') = \Pi(\vec{r}-\vec{r'};t-t')$ and the equality above is a convolution, from which it follows that in such systems:

$$\rho_{ind}(\vec{q},\omega) = e^2\Pi(\vec{q},\omega)\phi_{ext}(\vec{q},\omega)$$

showing that the charge susceptibility is $\chi(\vec{q},\omega) = e^2\Pi(\vec{q},\omega)$ and therefore something we can calculate.

Before doing this calculation for our jellium model, let me make a couple of general comments:

1. you can generalize this approach to calculate non-linear response functions, by (consistently) keeping higher order terms in the evolution operator and the expectation values.

2. this approach works for any kind of response function. For instance, if we apply an electric field $\vec{E}(\vec{r},t) = -\frac{\partial\vec{A}(\vec{r},t)}{\partial t}$, then this vector potential is coupled to the current density operator $\hat{j}(\vec{r})$, i.e. $\hat{H}_{ext}(t) = \int d\vec{r}\hat{j}(\vec{r})\vec{A}(\vec{r},t)$. The electric current will drive a current: $\delta\vec{j}(\vec{r},t) = \langle\Psi(t)|\hat{j}(\vec{r})|\Psi(t)\rangle - \langle\Psi_0|\hat{j}(\vec{r})|\Psi_0\rangle$. In the linear approximation, this allows us to calculate the conductivity from $\delta j_\alpha(\vec{q},\omega) = \sigma_{\alpha\beta}(\vec{q},\omega)E_\beta(\vec{q},\omega)$ to find $\sigma_{\alpha\beta}(\vec{q},\omega)$ as the Fourier transform of $\sigma_{\alpha\beta}(\vec{r}-\vec{r'};t-t') \sim -\frac{i}{\hbar}\theta(t-t')\langle\Psi_0|[\hat{j}_{\alpha,I}(\vec{r},t),\hat{j}_{\beta,I}(\vec{r'},t')]|\Psi_0\rangle$. Similarly, if the system is coupled to an external magnetic field, this will result in a magnetization from which we can define the magnetic susceptibility as the ratio between this induced magnetization and the applied magnetic field. The magnetic susceptibity is again proportional to one of these Green's functions, but now the commutator involves two magnetization operators, since this is what couples to the external (magnetic) field. I hope you get the idea. Again, this is something that is normally covered in much more detail in phys503.

3. so far, I have presented things like they are presented in all textbooks. I could just go on and you (like myself, when I was a graduate student) might not notice a big problem with what I just did, namely that I changed the definition of the susceptibility!

The correct definiton (see pg. 23) is $\rho_{ind} = \chi\phi_{tot}$, not the $\rho_{ind} = \chi\phi_{ext}$ used above! In fact, since $\phi_{ext} = \epsilon(\vec{q},\omega)\phi_{tot}$, we should decide from the RPA calculation that $e^2\Pi(\vec{q},\omega)\epsilon(\vec{q},\omega) = \chi(\vec{q},\omega)$. Using the link between ϵ and χ, this allows us to calculate χ, but it is obviously not $e^2\Pi(\vec{q},\omega)$.

It is a mystery to me why people claim that $\chi(\vec{q},\omega) = e^2\Pi(\vec{q},\omega)$ and why nobody else seems bothered by it. I will continue with this (wrong) formula because I should familiarize you with what is found in textbooks. Just keep this in mind if you ever need to do research involving screening, and if you so, then use the correct formula.

3.3 Screening in a free electron gas

To warm up, let us see what is the dielectric function in a free electron gas, i.e. if $\hat{H}_0 = \sum_{\vec{k},\sigma}\epsilon(k)c^\dagger_{\vec{k},\sigma}c_{\vec{k},\sigma}$. Then the GS is $|\Psi_0\rangle = \prod_{\vec{k}|<k_F,\sigma}c^\dagger_{\vec{k},\sigma}|0\rangle$ where $k_F = (3\pi^2 n)^{\frac{1}{3}}$. Comments: If you worry about how we keep the free electrons together, worry not - we put them inside a box of volume V so they cannot fly away. If you are confused about what gets screened if the electrons are non-interacting, the answer is the electric field produced by some external test charge. By this,

I mean some charge that is distinguishable from the electrons, and which can interact with the electrons even though we pretend that the electrons do not interact with one another.

We want to calculate the Fourier transform of $\Pi(\vec{r},t;\vec{r'},t') = -\frac{i}{\hbar}\theta(t-t')\langle\Psi_0|[\hat{n}_I(\vec{r},t),\hat{n}_I(\vec{r'},t')]|\Psi_0\rangle$; let's carefully calculate each quantity on its own. First, as we found out in a homework, in this basis $\hat{n}(\vec{r}) = \sum_{\vec{k},\vec{k'},\sigma}\frac{e^{-i(\vec{k}-\vec{k'})\vec{r}}}{V}c^\dagger_{\vec{k},\sigma}c_{\vec{k'},\sigma}$. We now have to take this into the interaction picture. Because our Hamiltonian is so simple, it is straightforward to check (check!) that $c_{I,\vec{k},\sigma}(t) = e^{-\frac{i}{\hbar}\epsilon(k)t}c_{\vec{k},\sigma}$ and $c^\dagger_{I,\vec{k},\sigma}(t) = e^{\frac{i}{\hbar}\epsilon(k)t}c^\dagger_{\vec{k},\sigma}$. So putting everything together, we find:

$$\hat{n}_I(\vec{r},t) = \sum_{\vec{k},\vec{k'},\sigma}\frac{e^{-i(\vec{k}-\vec{k'})\vec{r}}}{V}e^{\frac{i}{\hbar}(\epsilon(k)-\epsilon(k'))t}c^\dagger_{\vec{k},\sigma}c_{\vec{k'},\sigma}$$

Plugging this into the formula, we find that:

$$\Pi(\vec{r},t;\vec{r'},t') = -\frac{i}{\hbar}\theta(t-t')\sum_{\vec{k},\vec{k'},\sigma}\frac{e^{-i(\vec{k}-\vec{k'})\vec{r}}}{V}e^{\frac{i}{\hbar}(\epsilon(k)-\epsilon(k'))t}\sum_{\vec{k}_1,\vec{k'}_1,\sigma_1}\frac{e^{-i(\vec{k}_1-\vec{k'}_1)\vec{r'}}}{V}e^{\frac{i}{\hbar}(\epsilon(k_1)-\epsilon(k'_1))t'}$$

$$\times\langle\Psi_0|[c^\dagger_{\vec{k},\sigma}c_{\vec{k'},\sigma},c^\dagger_{\vec{k}_1,\sigma_1}c_{\vec{k'}_1,\sigma_1}]|\Psi_0\rangle$$

Now let's calculate the expectation value. Using the identity $[AB,C] = A[B,C]+[A,C]B$ and the anticommutation operators for the creation and annihilation operators, we find $[c^\dagger_{\vec{k},\sigma}c_{\vec{k'},\sigma},c^\dagger_{\vec{k}_1,\sigma_1}c_{\vec{k'}_1,\sigma_1}] = \delta_{\vec{k'},\vec{k}_1}\delta_{\sigma\sigma_1}c^\dagger_{\vec{k},\sigma}c_{\vec{k'}_1,\sigma} - \delta_{\vec{k},\vec{k'}_1}\delta_{\sigma\sigma_1}c^\dagger_{\vec{k}_1,\sigma}c_{\vec{k'},\sigma}$. The expectation value is simple, eg $\langle\Psi_0|c^\dagger_{\vec{k},\sigma}c_{\vec{k'}_1,\sigma}|\Psi_0\rangle = \delta_{\vec{k},\vec{k'}_1}n_{\vec{k},\sigma}$ where $n_{\vec{k},\sigma} = \theta(k_F - |\vec{k}|)$ is the occupation number of that state, 1 or 0 depending on whether k is below or above k_F. The second expectation value is similar and we now see that both terms contain the same δ-functions, which allow us to get rid of half of the sums, to find:

$$\Pi(\vec{r},t;\vec{r'},t') = -\frac{i}{\hbar}\theta(t-t')\sum_{\vec{k},\vec{k'},\sigma}\frac{e^{-i(\vec{k}-\vec{k'})(\vec{r}-\vec{r'})}}{V^2}e^{\frac{i}{\hbar}(\epsilon(k)-\epsilon(k'))(t-t')}\left(n_{\vec{k},\sigma}-n_{\vec{k'},\sigma}\right)$$

So we see that indeed, this quantity depends only on $t-t'$ and $\vec{r}-\vec{r'}$ as should be the case for homogeneous systems, and we can Fourier transform. Note that $\theta(t) = -\int_{-\infty}^{\infty}\frac{d\Omega}{2\pi i}\frac{e^{-i\Omega t}}{\Omega+i\eta}$, where $\eta\to 0$ is a small positive number. After some algebra, we finally find:

$$\chi^{(0)}(\vec{q},\omega) = e^2\Pi(\vec{q},\omega) = \frac{e^2}{V}\sum_{\vec{k},\sigma}\frac{n_{\vec{k},\sigma}-n_{\vec{k}+\vec{q},\sigma}}{\hbar\omega+\epsilon(\vec{k})-\epsilon(\vec{k}+\vec{q})+i\eta}$$

The upperscript 0 should remind us that this is the result for free electrons. In the literature, this result is referred to as **the Random Phase Approximation (RPA) formula**. I will comment more on this (confusing) name below.

It turns out that this function can also be evaluated analytically, but before analyzing its predictions about screening, let us quickly discuss what is the result for the jellium model.

3.4 Screening in the jellium model

At the HF level, you might be tempted to repeat the above calculation but now with $\hat{H}\approx\sum_{\vec{k},\sigma}E_k a^\dagger_{\vec{k},\sigma}a_{\vec{k},\sigma}$ corresponding to the HF "best guess". If you do that, everything goes the same,

except the one-particle energies are different, and you find:

$$\chi^g(\vec{q},\omega) = e^2\Pi(\vec{q},\omega) = \frac{e^2}{V}\sum_{\vec{k},\sigma}\frac{n_{\vec{k},\sigma} - n_{\vec{k}+\vec{q},\sigma}}{\hbar\omega + E_{\vec{k}} - E_{\vec{k}+\vec{q}} + i\eta}$$

This is referred to as the **generalized RPA**. This is no longer possible to evaluate analytically (because E_k are pretty complicated functions), so textbooks may mention it but use the RPA result from above to discuss screening in the jellium model. In the limit where the e-e interactions are weak (because the screening is very effective) this is a reasonable approximation because to zero order the two susceptibilities are the same and the first order correction should be small (plus, as I said, $\chi^{(0)}(\vec{q},\omega)$ can be calculated analytically, which is very useful to give us some intuition about what is happening). So we will do the same, but let me rant a bit first, because the generalized RPA is not the proper RPA for the jellium model, either. The problem is that when we add the external perturbation we should redo the self-consistent calculations, because the states of the electrons are affected by the external field and this changes their wavefunctions and eigenenergies from the HF values we obtained in the unperturbed case. Of course, the corrections are small but they turn out to be similar to the terms we kept when we did RPA (remember that there the wavefunction was perturbed out of its GS by the external field. So what I'm saying is that there is a second, comparable, contribution to that change coming from variations of the HF wavefunctions in response to the external field, which must be calculated self-consistently). Because of that, the end result is even more complicated than $\chi^g(\vec{q},\omega)$ and I've never seen any textbook bothering to even show that proper formula, nevermind to calculate it (numerically) and analyze its predictions.

I hope you will learn how to do proper RPA in Phys503, although chances are you will not have the time for that. I found D.J. Rowe's book that I already mentioned, and another book by Blaizot and Ripka, to contain the most clear explanations on the meaning of RPA – as the next bext approximation building on top of the HF – and how to do it properly. The first book focusses on equation-of-motion approaches, the second on variational approaches. They are equivalent but conceptually you may find one more appealing than the other.

Going back to the literature: many textbooks claim that $\chi^{(0)}(\vec{q},\omega)$ is the RPA for the jellium model because they start from the jellium Hamiltonian and then do so many additional ad-hoc approximations that the contributions from the e-e interactions are totally lost (but they don't realize it). Some of this may just be because this is not an active research area and each author just says whatever he/she was taught and doesn't bother thinking too carefully about it. I only discovered these differences because I needed RPA in my PhD work for more complicated Hamiltonians (like Hubbard) and so I had to dig a bit deeper to understand what it is and how to do it in a less "ad-hoc" manner. So if you will need to do RPA for your research, keep this in mind and learn to do proper RPA. End of rant.

Returning to $\chi^{(0)}(\vec{q},\omega)$, it can be calculated analytically, as I said. I won't write the full expression here because we won't use it (you should try to derive it and check against a textbook result, it's good practice with integrals). Instead, let us consider it in some limits and see what we can learn from these.

3.5 RPA vs Thomas-Fermi

In the static limit $\omega = 0$, we find:

$$\epsilon_{RPA}(\vec{q},\omega) = 1 - \frac{4\pi}{q^2}\chi^{(0)}(\vec{q},\omega) \to 1 - \frac{4\pi e^2}{Vq^2}\sum_{\vec{k},\sigma}\frac{n_{\vec{k},\sigma} - n_{\vec{k}+\vec{q},\sigma}}{\epsilon(\vec{k}) - \epsilon(\vec{k}+\vec{q}) + i\eta} = 1 + \frac{k_0^2}{q^2}F\left(\frac{q}{2k_F}\right)$$

where k_0 is the TF wavevector, and our good friend the Lindhart function has again made an appearance. Clearly, this answer agrees with $\epsilon_{TF}(q) = 1 + \frac{k_0^2}{q^2}$ in the limit when $q \ll k_F$ such that $F\left(\frac{q}{2k_F}\right) \to 1$. This is good, because this means that we are looking at screening at very long wavelengths, and that is where indeed we claimed that TF should be valid. For shorter wavelenghts, however, there is a difference between the two, so the quantum effects manifest themselves in the screening. The next figure shows a rough sketch of the difference in $1/\epsilon$ between the two models.

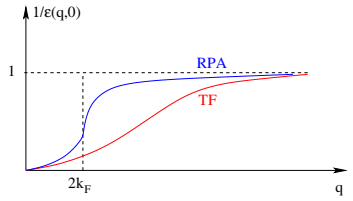

Figure 4: RPA vs TF static screening. Because of the Lindhart function, there is a singularity in the RPA response, but now at $2k_F$.

The RPA screens less (i.e., the screened potential is larger) than TF. Also note that at $q = 2k_F$ there is a sudden reduction in screening. This is due to the fact that states up to k_F are occupied and states above are empty. To create a low-energy (cheap) rearrangement in the electron density to screen out an external potential, we have to take an electron from just below the Fermi energy and excite it just above (so that it doesn't cost much energy). The largest momentum transfer we can get, therefore, is $2k_F$, which is why only potentials with momenta up to this value are screened efficiently. A more direct consequence of this can be observed in the form of the real space screened potential created by an external charge Q:

$$\phi_{tot}(\vec{r}) = \frac{1}{V}\int d\vec{q} e^{i\vec{q}\vec{r}} \frac{4\pi Q}{q^2 \epsilon_{RPA}(q,0)} \to \frac{\cos(2k_F r)}{(2k_F r)^3}$$

as $rk_F \to \infty$, i.e. at distance longer than the Fermi wavelength the screened potential oscillates! (and indeed vanishes much faster than $1/r$). This phenomenon is known as **Friedel oscillations** and because it is due to the sharpness of the Fermi surface, it is observed in all metals that are well described in terms of quasiparticles lying below the Fermi energy, i.e. in normal Fermi metals. We see these Friedel oscillations directly in STM images of an impurity placed on a metallic surface (google and look, if you haven't seen this before).

3.6 Plasma oscillations

Another limit that we can easily calculate is $q = 0$ (i.e., the homogenous case) for large $\omega \to \infty$. Here, we find (check!)

$$\epsilon_{RPA}(0,\omega) \to 1 - \frac{\omega_P^2}{\omega^2}$$

where

$$\omega_P = \sqrt{\frac{4\pi n e^2}{m}}$$

is the **plasma frequency**. This formula can also be obtained at a classical level, i.e. ignoring quantum effects, by considering how the liquid of electrons "sloshes" back and forth through the

background of positive charge in response to an external homogeneous ac electric field. I assume you have seen this simple calculation already (see any textbook) so I won't repeat it here.

This result explains why metals are shiny/reflective. Because the density n of electrons is large, the plasma frequency is usually big (tens of eV), meaning it is above the frequencies in the visible spectrum (1.5-3eV). Therefore, within the visible spectrum $\epsilon < 0$, which means that light with those frequencies cannot propagate inside the metal (remember that the index of refraction $= c/v = \sqrt{\epsilon}$ and here it would be an imaginary number, indicating attenuation instead of free propagation). Indeed, EM waves of such frequencies are reflected off the metal simply because their frequency is low enough that the electrons can respond to it and completely screen it. This is why metals such as Ag are used to make mirrors. For EM waves with much higher frequencies, the plasma oscillations are not fast enough to screen them out, so those waves can propagate inside the metal. However, they are usually absorbed fast because they can excite electron-hole pairs. Indeed, metals with ω_P below the visible spectrum look black because of this. One such example you are all familiar with is graphite, which we use in our pencils. It is a poor metal because it has a low n and therefore low ω_P, and indeed it is black. This makes it useful to write with (this plus the fact that it is made of very weakly coupled layers, so it can easily cleave under pressure to leave black traces on the paper).

3.7 Normal modes and collective excitations

Remember that $\phi_{tot}(\vec{q},\omega) = \phi_{ext}(\vec{q},\omega)/\epsilon(\vec{q},\omega)$. This means that if it is possible that $\epsilon(\vec{q},\omega) = 0$, then the system exhibits resonant behavior: no matter how small ϕ_{ext}, we have a diverging ϕ_{tot}. This signals the existence of **normal modes** for these $\vec{q},\omega$, i.e. at these energies and momenta, the system has its natural resonances. Of course, the ones we get from $\epsilon(\vec{q},\omega)$ are charge-related, i.e. they have to do with normal modes in the charge density. But similarly we could discuss magnetic normal modes, which appear from poles of the magnetic susceptibility, etc.

Let's consider the jellium model with its RPA (ahem) result and ask when $\epsilon_{RPA}(\vec{q},\omega) = 0$, in other words when:

$$1 = \frac{4\pi e^2}{q^2 V} \sum_{\vec{k},\sigma} \frac{n_{\vec{k},\sigma} - n_{\vec{k}+\vec{q},\sigma}}{\hbar\omega + \epsilon(\vec{k}) - \epsilon(\vec{k}+\vec{q}) + i\eta}$$

First, let us rewrite this in a more convenient form, by changing the sum over $\vec{k}$ into the second term to sum over $\vec{k'} = -(\vec{k}+\vec{q})$. This changes the denominator, while in the numerator now we have a simple Heaviside function, and we end up with:

$$1 = \frac{8\pi e^2}{\hbar q^2 V} \sum_{|\vec{k}|<k_F} \left[\frac{1}{\omega - \omega_{k,q}} - \frac{1}{\omega + \omega_{k,q}} \right]$$

where I'll use the shortand notation $\omega_{k,q} = \frac{1}{\hbar}[\epsilon(\vec{k}+\vec{q}) - \epsilon(\vec{k})] = \frac{\hbar}{2m}[2\vec{k}\vec{q} + q^2]$. Since $\vec{k}$ is inside the Fermi sphere, we have $\omega_{min}(q) \leq \omega_{k,q} \leq \omega_{max}(q)$, where $\omega_{min}(q) = \frac{\hbar}{2m}[-2k_F q + q^2], \omega_{max}(q) = \frac{\hbar}{2m}[2k_F q + q^2]$.

Suppose now that we fix a value of $\vec{q}$, and try to find $\omega > 0$ where that equation is obeyed (see sketch above, left). First, assume that V is finite, so that only certain $\vec{k}$ values are allowed. The function on the right diverges at each corresponding ω_{kq}, so there will be many solutions in the interval $\omega_{min}(q) \leq \omega_{k,q} \leq \omega_{max}(q)$, as sketched. In the limit $V \to \infty$, these solutions will merge in a continuum, i.e. for any ω in that range we will find a normal mode with that $\vec{q}$. These are

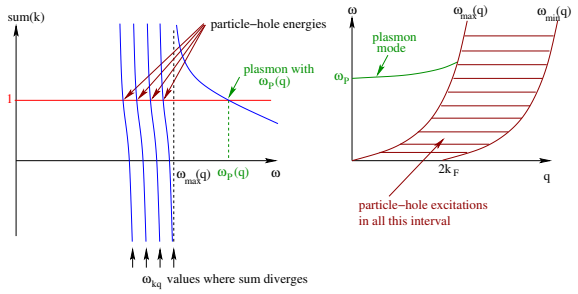

Figure 5: Left: geometric solution of equation $1 = \frac{8\pi e^2}{\hbar q^2 V} \sum_{|\vec{k}|<k_F} \left[\frac{1}{\omega - \omega_{k,q}} - \frac{1}{\omega + \omega_{k,q}} \right]$; the blue line sketches the function on the rhs. Right: the spectrum of the resulting normal modes.

called **particle-hole** excitations because essentially they correspond to exciting an electron from state $\vec{k}$ below the Fermi energy, to $\vec{k} + \vec{q}$ above, which is why the energy is (nearly) ω_{kq}.

However, there is one more solution. Once we're above $\omega_{max}(q)$, the function must decrease from the last singularity related to the highest energy particle-hole excitation. Each term in the sum goes like $1/\omega^2$ at very large ω and one can verify that the sign is positive, so there must be one more point where this function crosses 1. This is the **plasmon** of momentum $\vec{q}$ and with energy $\omega_P(\vec{q})$. This is a **collective excitation** because it involves exciting all the electrons, not just one (like the electron-hole pairs). The resulting spectrum is shown in the figure to the right. In the limit $q \to 0, \omega_P(\vec{q}) \to \omega_P$, the plasma frequency we discussed before (the fact that all electrons are involved in this normal mode is seen from its dependence of n, the electron density). You might want to have some fun and try to find $\omega_P(\vec{q})$ for small (but not zero) q, to verify that it indeed increases with q like showed there. Many textbooks show this calculation.

It is important to be able to calculate these normal modes because the system responds strongly at their energies/momenta, so they are easy to pick up in various experimental measurements. In other words, these predictions are something that can be compared against experiments relatively straightforwardly.

4 Fermi liquid theory

As discussed, the HF approximation says that the GS of the jellium (or any other interacting model) is a Fermi see of quasiparticles, each of which is moving in a self-consistent potential created by all the other quasiparticles. However, in reality there are remnant interactions between the quasiparticles, described by $\hat{H} - \hat{H}_{HF}$ (which is definitely not zero!). These interactions will scatter the quasiparticles from any one state into other states, so naively we might expect that this picture of a Fermi sea of quasiparticles is totally useless because if we wait long enough, the quasiparticles will be scrambled into other states, and which states are occupied will continue to change as scattering goes on and on.

Luckily, in a class of materials which we call **Fermi metals**, this is not the case, because the Pauli principle guarantees that these scattering times diverge for the quasiparticle in states near the Fermi energy (those which are at much lower energies are not very likely to scatter no matter what, because of energy conservation). To understand how this works, consider a Fermi sea of occupied states at $T = 0$, plus an extra quasiparticle of energy $E_1 > E_F$. This can scatter on any quasiparticle from the Fermi sea, eg. one with energy $E_2 < E_F$. The result is that the

two quasiparticles will change their energies to E_3, E_4 which are both above E_F since only those states are free. Now consider the conservation of energy $E_1 + E_2 = E_3 + E_4$ and momentum $\vec{k}_1 + \vec{k}_2 = \vec{k}_3 + \vec{k}_4$. Clearly, we must have $E_1 + E_2 > 2E_F$ else there are no available states for scattering. This means that state 2 can be any state just below E_F, specifically within the shell of thickness $(E_1 - E_F)$, i.e. the corresponding phase space is $\sim (E_1 - E_F)$. Similarly, we can argue that we have as many options to choose state 3 (but now in a similarly thin shell above the Fermi energy); the state 4 is fixed by the conservation laws. So the total phase space available scales like $(E_1 - E_F)^2$. From Fermi's golden rule, the scattering rate goes like $\frac{1}{\tau} \sim \frac{2\pi}{\hbar^2}|M|^2 \times$ phase space available, where M is an averaged matrix element that generally cannot vary fast with E_1. So at $T = 0$, we expect $\frac{1}{\tau} \sim (E - E_F)^2 \to 0$ if $E \to E_F$, i.e. quasiparticles near the Fermi energy are infinitely long-lived (they take forever to scatter out of their states). At finite T we know that some states within $k_B T$ of the Fermi energy become free (below) or occupied (above), so this gives a bit more available phase space for scattering. The end result, which can be justified with proper calculations, is that the scattering for a quasiparticle of energy E is:

$$\frac{1}{\tau} = a(E - E_F)^2 + b(k_B T)^2$$

The closer we are to E_F and the lower T is, the longer it will take for the quasiparticle to scatter into a different state. This is why so long as the typical processes we are interested in occur on a faster time-scale, it is a reasonable approximation to say that the quasiparticles occupy a Fermi sea.

Of course, this is a very simplistic discussion and a lot more needs to be said to justify things properly, and to understand how to use these ideas in a correct way. There is a very nice, short and clear discussion of **Landau's theory of Fermi liquids** (Landau was the one who put forward these ideas of a Fermi liquid, based on the notion of weakly-interacting quasiparticles) in A. J. Leggett, Rev. Mod. Phys. 47, 331 (1975). A much more in-depth discussion is available in the famous book by Pines and Nozieres, "Theory of Quantum Liquids".

Let me end this section saying that these ideas do NOT work for all interacting systems, not even all metallic ones. This is why you'll likely hear lots of talks about **non-Fermi metals**. These are metals where the quasiparticle concept is partially or totally suspect, for various reasons. At this time, we do not understand such systems, i.e. there is no cohesive theoretical framework to deal with them and no new paradigm to explain their behavior. Needless to say, what such systems have in common are strong interactions – so let's take a very quick look at some simple examples, to get a feeling for why strong interactions can change things so dramatically.