PX453 problems

*These problems are not for credit. You will get most from them by trying to solve them yourself first. Information that may prove useful in solving them is given at the end. The problems marked ** indicate questions, which are of significantly above-average difficulty or relate to non-examinable material. They deal with extensions and applications of the central material.*

Bosonic Field Operators

1. In the typed lecture notes you will find the demonstration that

$$\hat{H}(\hat{a}^\dagger)^n|0\rangle = \left(n + \frac{1}{2}\right)\hbar\omega_0(\hat{a}^\dagger)^n|0\rangle.$$

(In the lectures we looked explicitly only at the state $\hat{a}^\dagger|0\rangle$, which we showed had energy $3\hbar\omega_0/2$.)

Find the normalisation constant A for the state

$$|n\rangle = A(\hat{a}^\dagger)^n|0\rangle.$$

(Hint: Consider $\langle n|n\rangle = A^2\langle 0|\hat{a}^n(\hat{a}^\dagger)^n|0\rangle$. Taking account of the commutator, $[\hat{a}, \hat{a}^\dagger] = 1$, commute all the lowering operators to the right so that they act on and annihilate the ground state $|0\rangle$.)

$$\hat{a}^n(\hat{a}^\dagger)^n|0\rangle = \left(\hat{a}^{n-1}(\hat{a}^\dagger)^n\hat{a} + \hat{a}^{n-1}[\hat{a}, (\hat{a}^\dagger)^n]\right)|0\rangle = n\left(\hat{a}^{n-1}(\hat{a}^\dagger)^{n-1}\right)|0\rangle.$$

Any term with $\hat{a}$ acting on $|0\rangle$ vanishes as one cannot annihilate quanta in the ground state. The commutator $[\hat{a}, (\hat{a}^\dagger)^n] = n(\hat{a}^\dagger)^{n-1}$ as shown in the lecture notes. Now repeat the process to find

$$\hat{a}^n(\hat{a}^\dagger)^n|0\rangle = n!\,,$$

and hence $A = 1/\sqrt{n!}$.

2. As discussed in the lectures, time-dependence is attributed to state-functions in the Schrodinger picture:

$$|\psi(t)\rangle = \mathrm{e}^{-i\hat{H}t/\hbar}|\psi(0)\rangle \equiv \hat{U}(t)|\psi(0)\rangle.$$

In the Heisenberg picture the time-dependence is attributed to operators:

$$\hat{O}_H(t) = \hat{U}^\dagger(t)\hat{O}_S\hat{U}(t),$$

while the state-functions are time-independent. The subscripts denote the operators in the Heisenberg and Schrodinger pictures respectively.

In the Heisenberg picture, the raising and lowering operators become

$$\hat{a} \to \hat{A}(t) = \mathrm{e}^{i\hat{H}t/\hbar}\hat{a}\,\mathrm{e}^{-i\hat{H}t/\hbar} \quad \text{and} \quad \hat{a}^\dagger \to \hat{A}^\dagger(t) = \mathrm{e}^{i\hat{H}t}\hat{a}^\dagger\,\mathrm{e}^{-i\hat{H}t}.$$

We want to show that, for an oscillator with Hamiltonian $\hat{H} = \hbar\omega_0(\hat{a}^\dagger\hat{a} + 1/2)$,

$$\hat{A}(t) = \mathrm{e}^{i\hat{H}t/\hbar}\hat{a}\,\mathrm{e}^{-i\hat{H}t/\hbar} = \hat{a}\,\mathrm{e}^{-i\omega_0 t}.$$

(a) Show that

$$\frac{d\hat{A}}{dt} = i\,\mathrm{e}^{i\hat{H}t/\hbar}[\hat{H},\hat{a}]\mathrm{e}^{-i\hat{H}t/\hbar}.$$

(b) Compute the commutator in part (a).

(c) Integrate the result in part (a) to find the result required.

(d) Does the result seem natural?

(a) Apply the product rule. (If you are worried about doing calculus on operators, write the exponential as its Taylor series and then differentiate term by term.)

$$\frac{d\hat{A}}{dt} = \mathrm{e}^{i\hat{H}t/\hbar}\frac{i\hat{H}}{\hbar}\hat{a}\,\mathrm{e}^{-i\hat{H}t/\hbar} + \mathrm{e}^{i\hat{H}t}\hat{a}\frac{i\hat{H}}{\hbar}\mathrm{e}^{-i\hat{H}t/\hbar} = \frac{i}{\hbar}\mathrm{e}^{i\hat{H}t/\hbar}[\hat{H},\hat{a}]\mathrm{e}^{-i\hat{H}t/\hbar}$$

(b) The commutator

$$[\hat{H},\hat{a}] = \hbar\omega_0[(\hat{a}^\dagger\hat{a} + \frac{1}{2}),\hat{a}] = -\hbar\omega_0\hat{a}.$$

(c) Inserting the result from (b) into (a) gives

$$\frac{d\hat{A}}{dt} = -i\omega_0\mathrm{e}^{i\hat{H}t}\hat{a}\mathrm{e}^{-i\hat{H}t} = -i\omega_0\hat{A},$$

which can be integrated to give

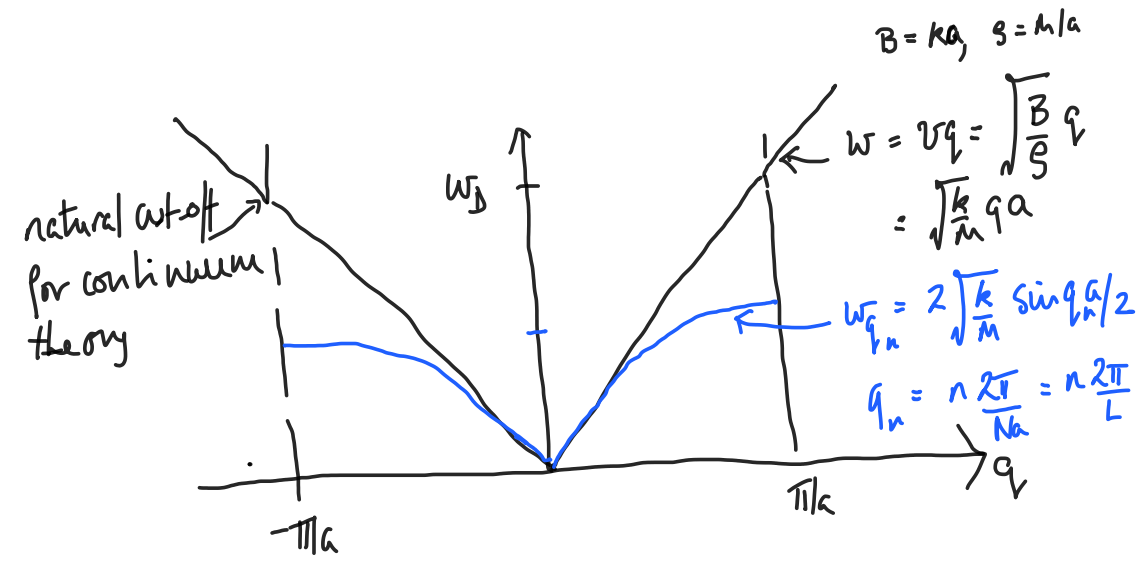
$$\hat{A}(t) = \hat{A}(0)\mathrm{e}^{-i\omega_0 t} = \hat{a}\mathrm{e}^{-i\omega_0 t}.$$

(d) If we imagine the operator $\hat{A}$ acting on a basis state, $|n\rangle$, then $\mathrm{e}^{-i\hat{H}t/\hbar}|n\rangle \sim \mathrm{e}^{-i\omega_n t}|n\rangle$. Apply the lowering operator to obtain $\sim \mathrm{e}^{-i\omega_n t}|n-1\rangle$. Now, when we apply $\mathrm{e}^{i\hat{H}t/\hbar}$, we obtain $\sim \mathrm{e}^{i\omega_{n-1}t - i\omega_n t}|n-1\rangle = \mathrm{e}^{-i\omega_0 t}|n-1\rangle$. The lowering operator has dropped the energy by $\hbar\omega_0$ and this is the origin the factor of $\mathrm{e}^{-i\omega_0 t}$ in the time-development of $\hat{a}$.

3. You should read Appendix A on the continuum limit of lattice oscillations. Check that you understand how the two treatments coincide for small q. Sketch the dispersion relation for both the microscopic model and the continuum limit.

The linear dispersion of the continuum model is also the basis of the so-called Debye model of lattice excitations. In this model, a cut-off frequency ω_D is introduced, so that excitations have frequencies between 0 and ω_D. Determine ω_D by requiring the number of modes to equal the number of ions.

The dispersion is sketched below. The two cases (microscopic theory in blue and continuum theory in black) agree for $|q| \to 0$, although not particularly well-drawn. The point is that the linear dependence continues to arbitrarily large q. This is correct as the continuum theory has infinitely many points on an interval of length L, so all q's are allowed.



In the Debye theory we cut off q at the Brillouin zone of the lattice. So at $q = \pi/a$. This gives $\omega_D = \pi\sqrt{k/m}$, while the maximum frequency in the microscopic model is $\omega_D = 2\sqrt{k/m}$.

Fermionic Field Operators

4. This question is designed to check that anticommutators are consistent with what we know about spin and statistics working from wavefunctions. Consider a system with two quantum states for fermions with creation operators $\hat{c}^\dagger_\uparrow$ and $\hat{c}^\dagger_\downarrow$, and basis states:

$$|0\rangle, |\uparrow\rangle = \hat{c}^\dagger_\uparrow|0\rangle, |\downarrow\rangle = \hat{c}^\dagger_\downarrow|0\rangle, \text{ and } |\uparrow\downarrow\rangle = \hat{c}^\dagger_\uparrow\hat{c}^\dagger_\downarrow|0\rangle.$$

If we were to work with state-functions, then

$$\hat{c}^\dagger_\uparrow\hat{c}^\dagger_\downarrow|0\rangle \to \frac{\uparrow_1\downarrow_2 - \uparrow_2\downarrow_1}{\sqrt{2}},$$

where we have adopted the convention that, in the two-particle state $\hat{c}^\dagger_{\uparrow_1}\hat{c}^\dagger_{\sigma_2}|0\rangle$, the sign of the amplitude of the product $\sigma_1\sigma_2$ (here $\sigma_1 = \uparrow$ and $\sigma_2 = \downarrow$) is positive. The amplitude for the state $\sigma_2\sigma_1$ follows from the requirement that we have to antisymmetrise over all assignments of particles to states (in this case there are only two).

(a) Explain why we are free to choose the overall sign of the wavefunction at will.

(b) Check that for all four states $|\psi\rangle$

$$\{\hat{c}^\dagger_{\sigma_1}, \hat{c}^\dagger_{\sigma_2}\}|\psi\rangle = 0.$$

a) The overall phase of a wavefunction is not a physical observable and contains no information relevant to the system's properties.

b) If $\sigma_2 = \sigma_1$, then the product $\hat{c}^\dagger_{\sigma_1}\hat{c}^\dagger_{\sigma_1}$ annihilates any state (it is not possible populate the state σ_1 with two fermions). In this case $\{\hat{c}^\dagger_{\sigma_1}, \hat{c}^\dagger_{\sigma_1}\}|\psi\rangle = 2\hat{c}^\dagger_{\sigma_1}\hat{c}^\dagger_{\sigma_1}|\psi\rangle = 0$ for any $|\psi\rangle$.

If $\sigma_1 \neq \sigma_2$, then $\hat{c}^\dagger_{\sigma_1}\hat{c}^\dagger_{\sigma_2}$ and $\hat{c}^\dagger_{\sigma_2}\hat{c}^\dagger_{\sigma_1}$ will annihilate the three states $|\uparrow\rangle, |\downarrow\rangle$ and $|\uparrow\downarrow\rangle$ as the product of the two operators will be trying to doubly-occupy at least one of the two

states. We only need to consider what happens when the product of the operators acts on the vacuum:

$$\hat{c}^\dagger_\uparrow \hat{c}^\dagger_\downarrow |0\rangle \to \frac{\uparrow_1\downarrow_2 - \uparrow_2\downarrow_1}{\sqrt{2}}, \quad \hat{c}^\dagger_\downarrow \hat{c}^\dagger_\uparrow |0\rangle \to -\frac{\uparrow_1\downarrow_2 - \uparrow_2\downarrow_1}{\sqrt{2}}$$
$$\Rightarrow \{\hat{c}^\dagger_\uparrow, \hat{c}^\dagger_\downarrow\}|0\rangle = 0$$

From now on, it is probably best to accept that the anticommutation recipe is the correct way to quantise fermionic fields rather than to work back from wavefunctions as here. Treat this as an axiom of the theory. In certain cases, like the Dirac equation in free space, it is possible to prove that this is the only way to quantise the theory consistently. (If you try to quantise the Dirac field as a Bose field, you quickly find contradictions.)

5. If we restrict to 1+1 dimensions (1 spatial and 1 temporal dimension) the Dirac equation for massless fermions can be written in a temporal or Weyl gauge, $A^0 = 0$, and with $c = 1$ and $q = -1$ as follows:

$$i\partial_0\psi_R = (-i\partial_1 - A^1)\psi_R, \quad \text{and} \quad i\partial_0\psi_L = (i\partial_1 + A^1)\psi_L.$$

In 1+1 dimensions, there are two-component spinors $(\psi_R, \psi_L)^t$ where t stands for transpose. There is not the idea of spin, which is associated with rotational symmetries which don't exist in 1D.

(a) In the absence of an em field we can take $A^1 = 0$. Check that any functions of the form

$$\psi_R(x - t) \quad \text{and} \quad \psi_L(x + t)$$

satisfy the respective equations. Which one is a right-mover and which a left-mover?

(b) Add back in the em-field, A^1, and show that both ψ_R and ψ_L satisfy conservation equations ($i = L, R$)

$$\partial_0\rho_i + \partial_1 j_i = 0$$

where $\rho_i = \psi_i^*\psi_i$ and find the corresponding currents j_i. Conclude that the numbers of right-movers and left-movers are independently conserved.

(c) Introduce a constant electric field $\dot{A}^1 = -E$ and set $A^1 = -Et$ ($E > 0$). Show that travelling wave solutions

$$\mathrm{e}^{ip(x-t) - iEt^2/2} \quad \text{and} \quad \mathrm{e}^{ip(x+t) + iEt^2/2}$$

exist for ψ_R and ψ_L respectively. The energy of the wave is given by ($\hbar = 1$) $\epsilon = i\partial_0$ acting on ψ. Show that the energy of the right-traveller varies in time as $p + Et$ and of the left-traveller as $-p - Et$. Show also that the momentum for the right mover, $-i\partial_1 - A^1$, varies $(p + Et)$.

(d) Now we come to the problem. We need to assume that all the states with negative energy are occupied. Explain why this together with your answer to the last part means that the number of right-movers increases with time and the number of left-movers decreases with time. The total charge should remain the same but the number of left- and right-movers is not conserved.

Congratulations, you have just discovered the chiral anomaly. Anomalies in QFT are related to quantities that are conserved classically but not conserved after quantisation. To make the theory work, we defined the vacuum to have all negative energy states occupied. When we shift the energy zero around with the electric field, we pull up and push down some states from/to this vacuum. These variations are in occupation numbers which we associate with particles (those with positive energy are particle states and empty states with negative energy are anti-particle states). This increase or decrease in the number of left- and right-movers has come from the infinity of negative energy states conveniently renamed the vacuum. This is the source of the non-conservation of left- and right-movers independently and is a genuine effect with experimental consequences.

The chiral anomaly is not restricted to 1D systems, but this 1D calculation illustrates its origin.

(a) Without the em field, the two equations are advection equations. Substituting the right-mover, $\psi_R(x-t)$, into the first equation we see that it is a solution. Similarly the left-mover satisfies the second equation.

The point of this question is to understand that in the classical limit these two equations appear to be independent of one another. After quantising, this is no longer the case. It is an example of an anomaly. In QFT, cases where some quantity is conserved classically (as Noether's theorem says it should be) but not after quantisation are called anomalies.

(b) If $\rho_R = \psi_R^*\psi_R$,

$$\partial_0\rho_R = \psi_R\partial_0\psi_R^* + \psi_R^*\partial_0\psi_R = \left(-\psi_R\partial_1\psi_R^* + \frac{A^1}{i}\psi_R^*\psi_R - \psi_R^*\partial_1\psi_R - \frac{A^1}{i}\psi_R^*\psi_R\right)$$
$$= \partial_1\psi_R^*\psi_R.$$

We identify $j_R = \psi_R^*\psi_R$. Not surprising really, as in the advection equation everything moves at constant speed. (Here the speed is 1.) For the left-movers $j_L = -\psi_L^*\psi_L$, with the minus sign indicating that the current is flowing to the left.

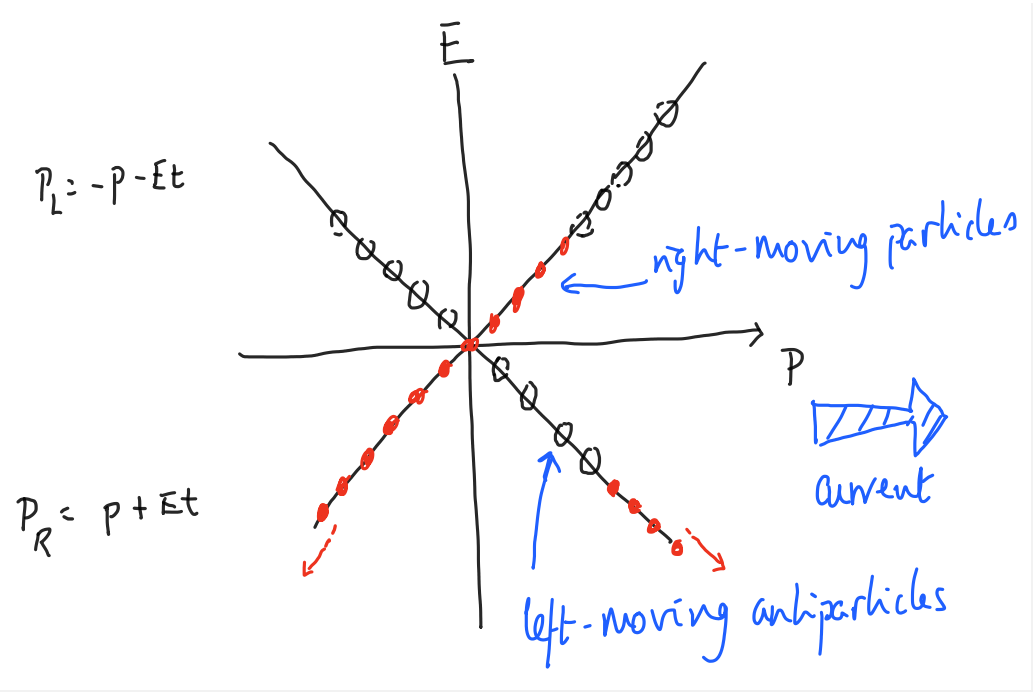
(c) Check first that the form given satisfies the equation

$$i\partial_0 \mathrm{e}^{ip(x-t)-iEt^2/2} = (p+Et)\,\mathrm{e}^{ip(x-t)-iEt^2/2} = (-i\partial_1 + Et)\,\mathrm{e}^{ip(x-t)-iEt^2/2}.$$

The energy (of any wavefunction) is $i\partial_0\psi$. We have just computed this and found $p+Et$. A similar calculation gives the energy of the left-mover to be $-p-Et$. These results are what you should expect. As the charged particle is accelerated (or decelerated) by the electric field its energy goes up (right-mover) or down (left-mover). The sign of E and the charge are, as usual, complicated by the convention that positively charged particles are accelerated in the direction of the electric field. Here we have assumed that the charge is -1 and the electric field is pointing in the negative direction.

What about the momentum? The momentum, $(-i\partial_1 + Et)\psi$, gives $p+Et$ for the right-moving case.

(d) As the electric field acts it pushes up the number of right-moving occupied states with energy above zero creating more (negatively-charged) right-movers. At the same time it pushes down the number of left-moving occupied states:



Those empty states with energy less than zero are interpreted as anti-particles or positively charged left-moving particles. The current due to the increased number of right-movers is exactly cancelled by the increased number of positively charged antiparticles moving to the left. So total charge is conserved but not that of right- and left-movers separately. This is an example of a phenomenon that arises when quantising fields. Sometimes the classically conserved quantities (for massless fermions these would be that total charge and the difference between the right-handed and left-handed particles are conserved) but the quantum theory cannot be set up to conserve both quantities.

Representations and Normalisations

(It is not essential to work through this question. It is here as a warning about the need to look out for different representations and different normalisations.)

6. One bugbear in this game is that there are different choices for the representation of the Dirac matrices and different normalisations for the spinors. Solutions and formulas for the same physical quantity can be different. People may choose the formulation which they think is best for illustrating some argument or for doing their sums. The two cases we will highlight are the representations of the Dirac matrices and the normalisations of the spinors.

(a) Consider the transformation (summation convention assumed)

$$\begin{aligned} \psi \to \tilde{\psi} = U\psi \quad \text{or in components} \quad & \tilde{\psi}_i = U_{ij}\psi_j \\ \boldsymbol{\alpha} \to \tilde{\boldsymbol{\alpha}} = U\boldsymbol{\alpha}U^\dagger \qquad\qquad\quad & \tilde{\alpha}^s_{il} = U_{ij}\alpha^s_{jk}U^\dagger_{kl} \\ \beta \to \tilde{\beta} = U\beta U^\dagger \qquad\qquad\quad & \tilde{\beta}_{il} = U_{ij}\beta_{jk}U^\dagger_{kl} \end{aligned} \tag{1}$$

Here U is a unitary matrix: $U^\dagger U = I$, where $U^\dagger$ is the Hermitian conjugate of U and $\tilde{H}$ is given by the expression for H with all quantities replaced by their transformed values. Show that if ψ is an eigenfunction of H with eigenvalue λ, *ie*

$$H\psi \equiv (-i\boldsymbol{\alpha}.\nabla + \beta m)\psi = \lambda\psi,$$

then

$$\tilde{H}\tilde{\psi} \equiv (-i\tilde{\boldsymbol{\alpha}}.\nabla + m\tilde{\beta})\tilde{\psi} = \lambda\tilde{\psi}.$$

$\tilde{\psi}$ is therefore an eigenvector of $\tilde{H}$ with the same eigenvalue as before. We obtain an equivalent description of the system using any choice of the matrices α and β related by a transformation of the type given in (1).

(b) Set the transformation matrix

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} \sigma^0 & \sigma^0 \\ \sigma^0 & -\sigma^0 \end{pmatrix},$$

and compute the corresponding $\tilde{\boldsymbol{\alpha}}$ and $\tilde{\beta}$. Take $\boldsymbol{\alpha}$ and β from the lecture notes (Handout 2 from the first part). You should find that $\tilde{\boldsymbol{\alpha}}$ is block diagonal. This representation of the Dirac matrices is called the chiral (or Weyl) representation as the solutions describe particles with different chirality. If the mass is zero these two chiral particles are not mixed by the Hamiltonian. You should also find that $\tilde{\beta}$ is block off-diagonal showing that the mass of the particle mixes the two independent particle states from the massless case.

(c) At various points the wavefunctions (solutions to the Dirac equation) have been quoted/derived. For example, the form for the positive energy solutions have been given as ($p_0 = E$, $\psi = \mathrm{e}^{-ip\cdot x}u^{(\sigma)}(\boldsymbol{p})$)

$$u^{(\sigma)}(\boldsymbol{p}) = \begin{pmatrix} \sqrt{\frac{p_0+m}{2m}}\phi^{(\sigma)} \\ \frac{\boldsymbol{\sigma}\cdot\boldsymbol{p}}{\sqrt{2m(p_0+m)}}\phi^{(\sigma)} \end{pmatrix}, \quad \tilde{u}^{(\sigma)}(\boldsymbol{p}) = \begin{pmatrix} \sqrt{p_0+m}\,\phi^{(\sigma)} \\ \frac{\boldsymbol{\sigma}\cdot\boldsymbol{p}}{\sqrt{(p_0+m)}}\phi^{(\sigma)} \end{pmatrix}.$$

In the notes of Tong, that we also referenced, you can find

$$\hat{u}^{(\sigma)}(\boldsymbol{p}) = \begin{pmatrix} (\sigma\cdot p)\,\phi^{(\sigma)} \\ m\,\phi^{(\sigma)} \end{pmatrix}, \quad \text{here} \quad \phi^{(1)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \phi^{(2)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Let's note the differences. The form $u^{(\sigma)}(\boldsymbol{p})$ is what was given in the representation of the operator $\hat{\psi}(x)$ in section 2.2 of the QFT notes which follows our main text Fradkin. $\tilde{u}^{(\sigma)}(\boldsymbol{p})$ is from handout 3 of part I of the module.

i. Check that $u^{(\sigma)}(\boldsymbol{p})$ and $\tilde{u}^{(\sigma)}(\boldsymbol{p})$ differ only by an overall factor and find this factor.

ii. (**) The function $\hat{u}^{(\sigma)}(\boldsymbol{p})$ looks more different. (Note that $\sigma\cdot p = \sigma^\mu p_\mu \neq \boldsymbol{\sigma}\cdot\boldsymbol{p}$.) What's going on? The point here is that Tong is working with the chiral representation of the Dirac equation (see around equation 4.18 in his notes).
Act on $\tilde{u}^{(\sigma)}(\boldsymbol{p})$ with the transformation matrix U given in part (b) and show that it is proportional to $\hat{u}^{(\sigma)}(\boldsymbol{p})$.

iii. Give the dimensions of the spinors listed above. (Remember that, with $\hbar = c = 1$, all dimensions are powers of energy.)

(a) Inserting for the transformed quantities gives

$$\begin{aligned}\tilde{H}\tilde{\psi} \equiv (-i\tilde{\boldsymbol{\alpha}}.\nabla + m\tilde{\beta})\tilde{\psi} &= (-iU\boldsymbol{\alpha}U^\dagger.\nabla + mU\beta U^\dagger)U\psi \\ &= U(-i\boldsymbol{\alpha}.\nabla + m\beta)\psi = U\lambda\psi = \lambda\tilde{\psi}.\end{aligned}$$

$\tilde{\psi}$ is an eigenvector of $\tilde{H}$ with the same eigenvalue as before.

(b)

$$\tilde{\beta} = U\,\alpha\,U^\dagger = \frac{1}{2}\begin{pmatrix} I & I \\ I & -I \end{pmatrix}\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\begin{pmatrix} I & I \\ I & -I \end{pmatrix} = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}$$

$$\tilde{\alpha} = U\,\alpha\,U^\dagger = \frac{1}{2}\begin{pmatrix} I & I \\ I & -I \end{pmatrix}\begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}\begin{pmatrix} I & I \\ I & -I \end{pmatrix} = \begin{pmatrix} \sigma & 0 \\ 0 & -\sigma \end{pmatrix}.$$

As mentioned in the question $\tilde{\alpha}$ is block diagonal. The two blocks are mixed by the matrix $\tilde{\beta}$. If the mass is zero this term drops out.

(c) i) $u^{(\sigma)}(\boldsymbol{p}) = \frac{1}{\sqrt{2m}}\tilde{u}^{(\sigma)}(\boldsymbol{p})$

(c) ii) If $A = (m + p_0 - \boldsymbol{\sigma}\cdot\boldsymbol{p})$ then $A^{-1} = \Delta^{-1}(m + p_0 + \boldsymbol{\sigma}\cdot\boldsymbol{p})$, with $\Delta = 2(m + p_0)m$. Define $s = \sqrt{2(p_0 + m)}$. Then

$$U\tilde{u}^{(\sigma)}(\boldsymbol{p}) = \frac{1}{s}\begin{pmatrix} (p_0 + m + \boldsymbol{\sigma}\cdot\boldsymbol{p})\,\phi^{(\sigma)} \\ (p_0 + m - \boldsymbol{\sigma}\cdot\boldsymbol{p})\,\phi^{(\sigma)} \end{pmatrix}$$

The "ratio" between the upper component and the lower component is

$$\begin{aligned}(p_0 + m - \boldsymbol{\sigma}\cdot\boldsymbol{p})^{-1}(p_0 + m + \boldsymbol{\sigma}\cdot\boldsymbol{p}) &= \frac{(p_0 + m)^2 + p^2 + 2(p_0 + m)\boldsymbol{\sigma}\cdot\boldsymbol{p}}{2(m + p_0)m} \\ &= \frac{1}{m}\left(p_0\sigma^0 + \boldsymbol{\sigma}\cdot\boldsymbol{p}\right) = \frac{1}{m}\sigma\cdot p\end{aligned}$$

as it is for $\hat{u}^{(\sigma)}(\boldsymbol{p})$.

(c) (iii) $[u] = E^0$, $[\tilde{u}] = E^{1/2}$ and $[\hat{u}] = E$. In practice, people would choose the representation/normalisation most appropriate for the aspect they are working on. For example, $u^{(\sigma)}(\boldsymbol{p})$ is the spinor which gives the expected 2-component spinor in the non-relativistic limit ($p_0 \approx m$). The spinor $\hat{u}^{(\sigma)}(\boldsymbol{p})$ is a natural starting point if $m = 0$. This is sometimes renormalised to

$$\hat{u}^{(\sigma)}(\boldsymbol{p}) = \begin{pmatrix} \sqrt{(\sigma\cdot p)}\,\phi^{(\sigma)} \\ \sqrt{(\sigma\cdot\bar{p})}\,\phi^{(\sigma)} \end{pmatrix}.$$

This has the same dimensions as $\tilde{u}$. For more on this, here's a video.

BCS Theory

7. In the notes we found the Bogoliubov transformation

$$\begin{pmatrix} \hat{\gamma}_{\boldsymbol{k},1} \\ \hat{\gamma}^\dagger_{\boldsymbol{k},2} \end{pmatrix} = U \begin{pmatrix} \hat{c}_{\boldsymbol{k},\uparrow} \\ \hat{c}^\dagger_{-\boldsymbol{k},\downarrow} \end{pmatrix} \equiv \begin{pmatrix} u_{\boldsymbol{k}} & -v_{\boldsymbol{k}} \\ v^*_{\boldsymbol{k}} & u^*_{\boldsymbol{k}} \end{pmatrix} \begin{pmatrix} \hat{c}_{\boldsymbol{k},\uparrow} \\ \hat{c}^\dagger_{-\boldsymbol{k},\downarrow} \end{pmatrix}$$
$$\begin{pmatrix} \hat{c}_{\boldsymbol{k},\uparrow} \\ \hat{c}^\dagger_{-\boldsymbol{k},\downarrow} \end{pmatrix} = U^\dagger \begin{pmatrix} \hat{\gamma}_{\boldsymbol{k},1} \\ \hat{\gamma}^\dagger_{\boldsymbol{k},2} \end{pmatrix} \equiv \begin{pmatrix} u^*_{\boldsymbol{k}} & v_{\boldsymbol{k}} \\ -v^*_{\boldsymbol{k}} & u_{\boldsymbol{k}} \end{pmatrix} \begin{pmatrix} \hat{\gamma}_{\boldsymbol{k},1} \\ \hat{\gamma}^\dagger_{\boldsymbol{k},2} \end{pmatrix},$$

with $u_{\boldsymbol{k}} = \cos\theta_{\boldsymbol{k}} \mathrm{e}^{i\phi_{\boldsymbol{k}}/2}$, $v_{\boldsymbol{k}} = \sin\theta_{\boldsymbol{k}} \mathrm{e}^{-i\phi_{\boldsymbol{k}}/2}$. The choice

$$\sin 2\theta_{\boldsymbol{k}} = \frac{|\Delta|}{\sqrt{\xi^2_{\boldsymbol{k}} + |\Delta|^2}}, \quad \cos 2\theta_{\boldsymbol{k}} = \frac{\xi_k}{\sqrt{\xi^2_{\boldsymbol{k}} + |\Delta|^2}}, \quad \phi_k = \phi,$$

diagonalised the Hamiltonian. Here $\Delta = |\Delta|\mathrm{e}^{i\phi}$ and $\xi_k = \epsilon_k - \mu$ with μ the chemical potential.

(a) Could we have assumed Δ to be real and not had to bother with complex amplitudes for $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$? (This is not a trick question.)

(b) Sketch $|u_{\boldsymbol{k}}|^2$ and $|v_{\boldsymbol{k}}|^2$ as a function of $k = |\boldsymbol{k}|$. Mark the chemical potential. (You should be able to do this from the limiting cases quoted in the lecture notes $\xi_k \to \pm\infty$ and $\xi_k = 0$ given in the lecture module.)

(c) In the limit $|\Delta| \to 0$, check that the Bogoliubov the creation operator $\hat{\gamma}^\dagger_{\boldsymbol{k},2} \sim \hat{c}^\dagger_{-\boldsymbol{k},\downarrow}$ for $\xi_{\boldsymbol{k}} > 0$ and $\hat{\gamma}^\dagger_{\boldsymbol{k},2} \sim c_{\boldsymbol{k},\uparrow}$ for $\xi_{\boldsymbol{k}} < 0$. In other words $\hat{\gamma}^\dagger_{\boldsymbol{k},2}$ makes a hole excitation below the Fermi energy and particle excitation above the Fermi energy. It is the equivalent of what we did in the Dirac equation in section 2.2 (the $\hat{b}^\dagger_\sigma(\boldsymbol{p})$ operators created particles and the $\hat{d}^\dagger_\sigma(\boldsymbol{p})$ operators created antiparticles).

(d) Sketch the density of states we derived in lectures for the BCS state.

(e) With the opening of the gap, one can think of occupied states below the chemical potential at $\xi_k = \epsilon_k - \mu$ shifting to $E_k = -\sqrt{\xi^2_{\boldsymbol{k}} + |\Delta|^2}$. If ν_F is the density of states at the Fermi energy in the normal state, we can think of $\sim \nu_F|\Delta|$ states being affected (per unit volume). Estimate a mean reduction in energy and hence the "condensation energy" of the superconducting ground state. (The condensation energy is the energy difference between the superconducting ground state and the normal state.)

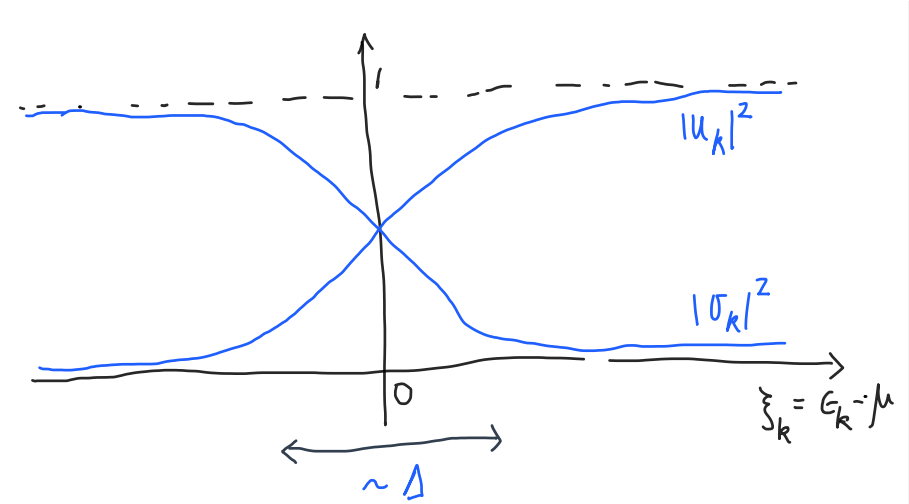
(f) (**) Compute the condensation energy in the BCS theory. This is the energy difference

$$E_{\mathsf{Cond}} = \langle FS|H_{BCS}|FS\rangle - \langle BCS|H_{BCS}|BCS\rangle$$

Note that it is important to use the same (approximate) Hamiltonian for both states. (The ** is a warning that the integrals involved are tedious and it is easy to lose track of things.)

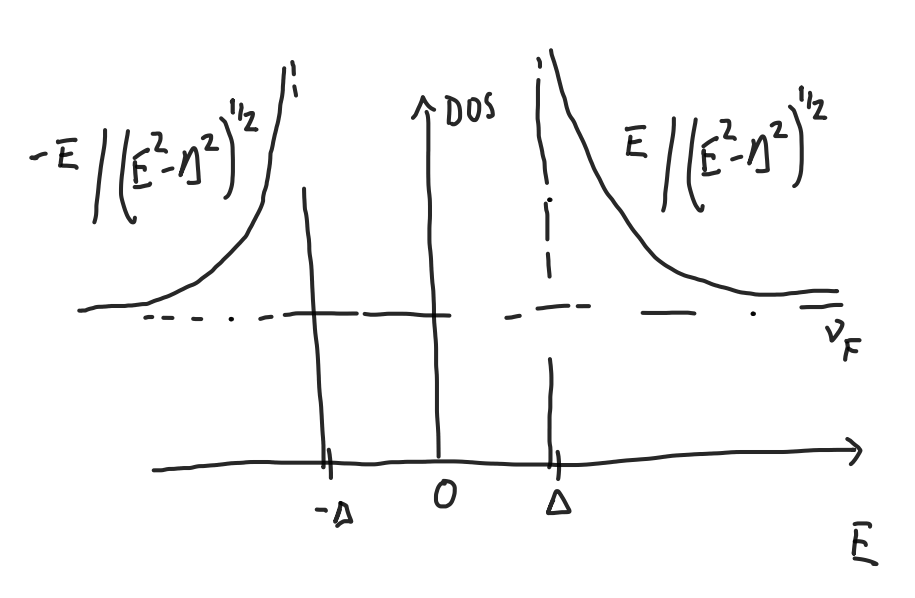
(a) Yes, we could have ignored the phase. This is because we are only considering a homogeneous system. However, in any case where currents flow, the phase will vary as a function of position and must be retained.

(b) We found that u_k tended to 1 for $\zeta_k \gg \mu$ and tended to 0 for $\zeta_k \ll \mu$. The energy scale on which these changes occur is set by $|\Delta|$.

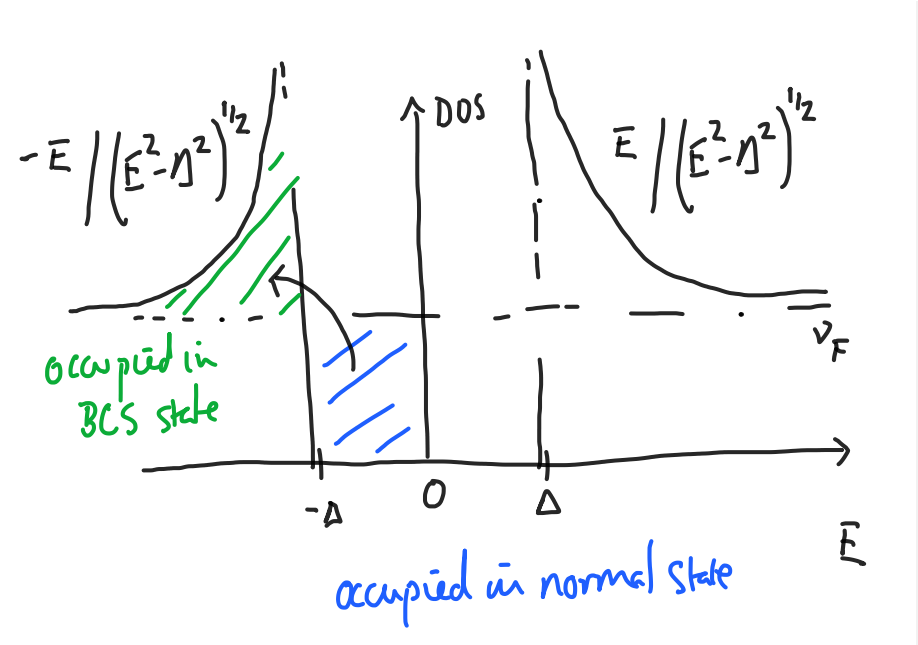


(c) $E_{\boldsymbol{k}}$ is always a positive energy, *ie* we always take the positive value of $\sqrt{\xi_{\boldsymbol{k}}^2 + |\Delta|^2}$. This means that both particle and anti-particle have positive energy.

(d) The DoS of the BCS state has has singularities at $E = \pm|\Delta|$.



(e) Spectral weight present in the normal state between $\pm|\Delta|$ has been shifted to energies below $-|\Delta|$ and above $|\Delta|$.



If $\nu_F\Delta$ states move down an average of $\Delta/2$ in energy. The total energy released as the system condenses into the BCS state is $\sim \nu_F\Delta^2/2$. We can be a more quantitative than this (see part (d)). However, we should be careful. The BCS state is derived using a mean-field treatment of the Hamiltonian. If we compute differences between different candidate ground states (in this case the BCS state and the filled Fermi sea), will be larger.

(f) The BCS Hamiltonian is

$$\hat{H} - \mu\hat{N} = \sum_{\boldsymbol{k},\tau} E_k \hat{\gamma}^\dagger_{\boldsymbol{k},\tau}\hat{\gamma}_{\boldsymbol{k},\tau} + \sum_{\boldsymbol{k}}(\xi_k - E_k).$$

This gives $\langle BCS|H_{BCS}|BCS\rangle = 0$, where we have dropped the constant (which is the same for both states).

The Bogoliubov transformation

$$\begin{pmatrix} \hat{\gamma}_{\boldsymbol{k},1} \\ \hat{\gamma}^\dagger_{\boldsymbol{k},2} \end{pmatrix} = U \begin{pmatrix} \hat{c}_{\boldsymbol{k},\uparrow} \\ \hat{c}^\dagger_{-\boldsymbol{k},\downarrow} \end{pmatrix} \equiv \begin{pmatrix} u_{\boldsymbol{k}} & -v_{\boldsymbol{k}} \\ v^*_{\boldsymbol{k}} & u^*_{\boldsymbol{k}} \end{pmatrix} \begin{pmatrix} \hat{c}_{\boldsymbol{k},\uparrow} \\ \hat{c}^\dagger_{-\boldsymbol{k},\downarrow} \end{pmatrix}$$

allows us to write the $\hat{\gamma}$ operators in terms of the free fermion operators, $\hat{c}$. Take $\phi_k = 0$ and identify energies by $k = |\boldsymbol{k}|$. Find (the factor of 2 is from the sum $\tau = 1, 2$)

$$\begin{aligned}
\langle FS|H_{BCS}|FS\rangle &= 2\sum_{\xi_k<0} E_k u_k^2 + 2\sum_{\xi_k>0} E_k v_k^2 \\
&= \sum_{\xi_k<0} E_k(1+\cos 2\theta_k) + \sum_{\xi_k>0} E_k(1-\cos 2\theta_k) \\
&= \sum_{\xi_k<0} E_k\left(1+\frac{\xi_k}{E_k}\right) + \sum_{\xi_k>0} E_k\left(1-\frac{\xi_k}{E_k}\right) = 2\sum_{\xi_k>0}\sqrt{\xi_k^2+\Delta^2} - \xi_k \\
&= 2\nu_F \int_0^X dx\, \left(\sqrt{x^2+\Delta^2} - x\right).
\end{aligned}$$

Here $X \gg \Delta$ is some bandwidth cutoff. With the substitution $x = \Delta \sinh u$ and $Y = \operatorname{arcsinh} X/\Delta$ gives

$$\begin{aligned}\langle FS|H_{BCS}|FS\rangle &= -\nu_F\left(\frac{X^2}{2} - \Delta^2\int_0^Y du\cosh^2 u\right)\\ &\approx \nu_F\left(\frac{X^2}{2} - \Delta^2\left[\frac{\mathrm{e}^{2u}}{2}\right]_0^Y\right) \approx \frac{\nu_F\Delta^2}{2}.\end{aligned}$$

In the final line we have used that $\cosh u \approx \sinh u \approx \mathrm{e}^u$ in the integral and $\Delta^2\mathrm{e}^{2Y} \approx X^2$.

The answer to part (d) is the important one to understand.

8. In the lectures we required that acting on the state

$$|\psi\rangle = p\,|0\rangle + q\,\hat{c}^\dagger_{\boldsymbol{k},\uparrow}|0\rangle + r\,\hat{c}^\dagger_{-\boldsymbol{k},\downarrow}|0\rangle + s\,\hat{c}^\dagger_{\boldsymbol{k},\uparrow}\hat{c}^\dagger_{-\boldsymbol{k},\downarrow}|0\rangle$$

with the operators $\hat{\gamma}_i$ should annihilate the state for all k. We argued that this meant that the BCS wavefunction was given by

$$|BCS\rangle = \prod_{\boldsymbol{k}}(u_{\boldsymbol{k}} + v_{\boldsymbol{k}}\hat{c}^\dagger_{\boldsymbol{k},\uparrow}\hat{c}^\dagger_{-\boldsymbol{k},\downarrow})|0\rangle.$$

Here

$$\begin{pmatrix}\hat{\gamma}_{\boldsymbol{k},1}\\ \hat{\gamma}^\dagger_{\boldsymbol{k},2}\end{pmatrix} = U\begin{pmatrix}\hat{c}_{\boldsymbol{k},\uparrow}\\ \hat{c}^\dagger_{-\boldsymbol{k},\downarrow}\end{pmatrix} \equiv \begin{pmatrix}u_{\boldsymbol{k}} & -v_{\boldsymbol{k}}\\ v^*_{\boldsymbol{k}} & u^*_{\boldsymbol{k}}\end{pmatrix}\begin{pmatrix}\hat{c}_{\boldsymbol{k},\uparrow}\\ \hat{c}^\dagger_{-\boldsymbol{k},\downarrow}\end{pmatrix}.$$

(a) Work through this argument to convince yourself that you can get the right result.

(b) Verify that the BCS wavefunction is normalised.

(a) Act with $\hat{\gamma}_{\boldsymbol{k},\tau}$ on $|\psi\rangle$ gives, using the anticommutation relations for the $\hat{c}_{\boldsymbol{k},\sigma}$ operators and the fact that $\hat{c}_{\boldsymbol{k},\sigma}|0\rangle = 0$:

$$\begin{aligned}\hat{\gamma}_{\boldsymbol{k},1}|\psi\rangle &= \left(u_{\boldsymbol{k}}\hat{c}_{\boldsymbol{k},\uparrow} - v_{\boldsymbol{k}}\hat{c}^\dagger_{-\boldsymbol{k},\downarrow}\right)\left(p\,|0\rangle + q\,\hat{c}^\dagger_{\boldsymbol{k},\uparrow}|0\rangle + r\,\hat{c}^\dagger_{-\boldsymbol{k},\downarrow}|0\rangle + s\,\hat{c}^\dagger_{\boldsymbol{k},\uparrow}\hat{c}^\dagger_{-\boldsymbol{k},\downarrow}|0\rangle\right)\\ &= u_{\boldsymbol{k}}q\,|0\rangle + u_{\boldsymbol{k}}s\,\hat{c}^\dagger_{-\boldsymbol{k},\downarrow}|0\rangle - v_{\boldsymbol{k}}p\,\hat{c}^\dagger_{-\boldsymbol{k},\downarrow}|0\rangle + v_{\boldsymbol{k}}q\,\hat{c}^\dagger_{\boldsymbol{k},\uparrow}\hat{c}^\dagger_{-\boldsymbol{k},\downarrow}|0\rangle,\\ \hat{\gamma}_{\boldsymbol{k},2}|\psi\rangle &= \left(+v_{\boldsymbol{k}}\hat{c}^\dagger_{\boldsymbol{k},\uparrow} + u_{\boldsymbol{k}}\hat{c}_{-\boldsymbol{k},\downarrow}\right)\left(p\,|0\rangle + q\,\hat{c}^\dagger_{\boldsymbol{k},\uparrow}|0\rangle + r\,\hat{c}^\dagger_{-\boldsymbol{k},\downarrow}|0\rangle + s\,\hat{c}^\dagger_{\boldsymbol{k},\uparrow}\hat{c}^\dagger_{-\boldsymbol{k},\downarrow}|0\rangle\right)\\ &= +v_{\boldsymbol{k}}p\,\hat{c}^\dagger_{\boldsymbol{k},\uparrow}|0\rangle + v_{\boldsymbol{k}}r\,\hat{c}^\dagger_{\boldsymbol{k},\uparrow}\hat{c}^\dagger_{-\boldsymbol{k},\downarrow}|0\rangle + u_{\boldsymbol{k}}r\,|0\rangle - u_{\boldsymbol{k}}s\,\hat{c}^\dagger_{\boldsymbol{k},\uparrow}|0\rangle.\end{aligned}$$

These both vanish if $q = r = 0$, while $p \propto u_{\boldsymbol{k}}$ and $s \propto v_{\boldsymbol{k}}$. Taking the product over $\boldsymbol{k}$ gives the BCS wavefunction.

(b) If it is normalised for each $\boldsymbol{k}$, the product (over all $\boldsymbol{k}$) state is normalised. Looking at a particular $\boldsymbol{k}$ gives (here $|0\rangle$ is the empty state)

$$\langle 0|(u^*_{\boldsymbol{k}} - v^*_{\boldsymbol{k}}\hat{c}_{-\boldsymbol{k},\downarrow}\hat{c}_{\boldsymbol{k},\uparrow})(u_{\boldsymbol{k}} - v_{\boldsymbol{k}}\hat{c}^\dagger_{\boldsymbol{k},\uparrow}\hat{c}^\dagger_{\boldsymbol{k},\downarrow})|0\rangle = |u_{\boldsymbol{k}}|^2 + |v_{\boldsymbol{k}}|^2 = 1. \quad (2)$$

Interacting Electrons

9. We would like to estimate the ratio r_s/a for the three elements sodium, potassium and copper. Sodium and potassium have the BCC structure and copper the FCC structure.

(a) The lattice constants for the three elements are 4.3Å (Na), 3.6Å (Cu) and 5.33Å (K). Find the volume of the unit cell for the three elements and give the number of ions per unit cell.

(b) Estimate the conduction electron density assuming the each ion gives one conduction electron.

(c) Find r_s in units of the Bohr radius $a = 0.5294$Å.

(d) Comment on the results.

		Answer to part	a)		b)			c)
			m^3		m^(-3)	metres		
	Lattice	a	V	N	Density	rs	a	rs/a
Na	BCC	4.3	7.9507E-29	2	2.52E+28	2.12E-10	5.29E-11	4.0
Cu	FCC	3.6	4.6656E-29	4	8.57E+28	1.41E-10	5.29E-11	2.7
K	BCC	5.328	1.5125E-28	2	1.32E+28	2.62E-10	5.29E-11	5.0

d) These values are between 1 and 6 as we stated in the lecture notes and suggest that interaction effects should be at least as important as the kinetic energy. Yet models based on free electron theory work well for these materials. We attribute the success of the theories to screening (the electrons collectively screen the Coulomb interactions between electrons). There are also arguments due to Landau explaining why a free electron model should work in the presence of interactions (look up Landau Fermi Liquid theory for more on this).

10. Here we will find the exact eigenstates of the Hubbard Hamiltonian (see Appendix D in the notes) in a two-site problem,

$$\hat{H} = \sum_{\sigma} \left[t(\hat{c}^{\dagger}_{1\sigma}\hat{c}_{2\sigma} + \hat{c}^{\dagger}_{2\sigma}\hat{c}_{1\sigma}) \right] + U\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow}.$$

The idea of this model is to include an important bit of the Coulomb repulsion namely the interaction energy of two electrons (with opposite spins) in the same orbital. This interaction is expected to be most important in spatially localised orbitals, like d or f orbitals. If this orbital is doubly-occupied, two electrons are always close to one another and hence their interaction is large. This is also the reason that magnetism and magnetic phenomena are often found in materials containing transition metal ions or lanthanide ions.

(a) Verify that the following are eigenstates for the system with 1 electron

$$|\pm,\sigma\rangle_1 = \frac{(\hat{c}^{\dagger}_{1,\sigma} \pm \hat{c}^{\dagger}_{2,\sigma})}{\sqrt{2}}|0\rangle.$$

Do the same for the eigenstates of the system with three electrons

$$|\pm,\sigma\rangle_3 = \hat{c}^{\dagger}_{1,-\sigma}\hat{c}^{\dagger}_{2,-\sigma}|\pm,\sigma\rangle_1.$$

(b) For systems with two electrons, explain why we need only consider the two separate groups of states

$$1.\quad \hat{c}^\dagger_{1\uparrow}\hat{c}^\dagger_{1\downarrow}|0\rangle, \quad \hat{c}^\dagger_{2\uparrow}\hat{c}^\dagger_{2\downarrow}|0\rangle \quad \text{and} \quad \frac{\hat{c}^\dagger_{1\uparrow}\hat{c}^\dagger_{2\downarrow}-\hat{c}^\dagger_{1\downarrow}\hat{c}^\dagger_{2\uparrow}}{\sqrt{2}}|0\rangle$$

and

$$2.\quad \hat{c}^\dagger_{1\uparrow}\hat{c}^\dagger_{2\uparrow}|0\rangle, \quad \frac{\hat{c}^\dagger_{1\uparrow}\hat{c}^\dagger_{2\downarrow}+\hat{c}^\dagger_{1\downarrow}\hat{c}^\dagger_{2\uparrow}}{\sqrt{2}}|0\rangle \quad \text{and} \quad \hat{c}^\dagger_{1\downarrow}\hat{c}^\dagger_{2\downarrow}|0\rangle.$$

(If you can't find the general argument immediately, simply act on these states with the Hamiltonian and see what comes out.)

(c) The second group of states in part (b) are already eigenstates of $\hat{H}$. Find their energies.

(d) Show that the Hamiltonian has matrix elements in the first group of states:

$$H_{ij} = \begin{pmatrix} U & 0 & \sqrt{2}t \\ 0 & U & \sqrt{2}t \\ \sqrt{2}t & \sqrt{2}t & 0 \end{pmatrix}.$$

Here $H_{ij} = \langle i|\hat{H}|j\rangle$ where $|i\rangle$ denotes one of the three states in the group. Find the eigenvalues of this matrix. (Although this will give you a cubic equation to solve you should find that the eigenvalue $\epsilon = U$ factors out trivially leaving only a simple quadratic.)

(e) Consider the limit $U/|t| \gg 1$ and find an expression for the lowest energy state in part (d). In Appendix D an estimate is given for the difference between this state and the triplet states considered in part (c) based on second order perturbation theory. Verify that your answers in the regime U/t large.

(a) Act on the one-electron states with the Hamiltonian:

$$\begin{aligned}\hat{H}|\pm,\sigma\rangle_1 &= \left[\sum_\sigma t(\hat{c}^\dagger_{1\sigma}\hat{c}_{2\sigma}+\hat{c}^\dagger_{2\sigma}\hat{c}_{1\sigma}) + U\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow}\right]\frac{(\hat{c}^\dagger_{1,\sigma}\pm\hat{c}^\dagger_{2,\sigma})}{\sqrt{2}}|0\rangle \\ &= \pm t\frac{(\hat{c}^\dagger_{1,\sigma}\pm\hat{c}^\dagger_{2,\sigma})}{\sqrt{2}}|0\rangle = \pm t\,|\pm,\sigma\rangle_1.\end{aligned}$$

The states have energies $\pm t$. The term proportional to t is called the hopping term. It shifts an electron from the orbital on site 1 to site 2 and vice versa. As there is only one electron the terms proportional to U annihilate the states.

The states with three electrons have energy $U \pm t$. The states with opposite spin to σ are occupied on both sites. The hopping term shifts the electron with spin σ to the neighbouring site but cannot move electrons with spin $-\sigma$ as the corresponding orbital on the neighbouring site is occupied.

(b) The states in group 1 are spin singlet states ($S = 0$) while the states in group 2 are spin triplet states ($S = 1$). Although we haven't shown this explicitly, the Hamiltonian is invariant under changes of the spin direction (no direction in the spin space is special).

Consequently the Hamiltonian cannot have non-zero matrix elements between states with different total spin.

(c) The states all have energy zero. The Hamiltonian annihilates all of the states: there are no doubly occupied sites, while the hopping term cannot move one electron to the neighbouring site as the orbital is occupied.

(d) Eigenvalues found as follows

$$\begin{aligned}
0 &= \begin{vmatrix} U-\lambda & 0 & \sqrt{2}t \\ 0 & U-\lambda & \sqrt{2}t \\ \sqrt{2}t & \sqrt{2}t & -\lambda \end{vmatrix} = (U-\lambda)\left[(U-\lambda)(-\lambda) - 2t^2\right] - 2t^2(U-\lambda) \\
&= (U-\lambda)(\lambda^2 - U\lambda - 4t^2) \\
&= (U-\lambda)\left[\left(\lambda - \frac{U}{2}\right)^2 - \left(\frac{U}{2}\right)^2 - 4t^2\right] \\
&= (U-\lambda)\left(\lambda - \left(\frac{U}{2} - \sqrt{\left(\frac{U}{2}\right)^2 + 4t^2}\right)\right)\left(\lambda - \left(\frac{U}{2} + \sqrt{\left(\frac{U}{2}\right)^2 + 4t^2}\right)\right).
\end{aligned}$$

We can read off the eigenvalues as the three zeros of this cubic expression.

(e) In the limit of large U, the lowest energy states has

$$\epsilon = \frac{U}{2} - \frac{U}{2}\left(1 + \frac{4t^2}{(U/2)^2}\right)^{1/2} \approx -\frac{4t^2}{U}.$$

This is the energy obtained using second order perturbation theory (see appendix D). The quantity $4t^2/U$ is usually denoted by J as the Hamiltonian for the four low energy states is equivalent to that of a spin interaction.

11. An early treatment of interacting electrons is that of the Hartree approximation. For the free electron gas it is quite simple. The Hamiltonian is

$$\hat{H} = \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}} \hat{c}^\dagger_{\boldsymbol{k},\sigma} \hat{c}_{\boldsymbol{k},\sigma} + \frac{1}{2}\sum_{\boldsymbol{q}} v(q)\hat{\rho}(\boldsymbol{q})\hat{\rho}(-\boldsymbol{q}) - v(0)n_0\hat{\rho}(0) + V_{bb}.$$

Here the last two terms are the attractive interaction of the electrons with a constant positive charged background charge density n_0 and the self-interaction of the background charge (note that this is not an extensive term and is usually not considered). The interaction $v(q) \sim 1/q^2$ is the Fourier transform of the Coulomb interaction. The energies $\epsilon_{\boldsymbol{k}} = \hbar^2 k^2/2m$.

We will assume that the vacuum is the filled Fermi sea $|\psi_0\rangle = \prod_{k<k_F}(\hat{c}^\dagger_{\boldsymbol{k},\uparrow}\hat{c}^\dagger_{\boldsymbol{k},\downarrow})|0\rangle$. In the following assume that expectation values of operators are with respect to this filled Fermi sea.

a) Why is $n_0 = <\hat{\rho}(0)>$? Work from the definition $\hat{\rho}(0) = \frac{1}{V}\int_V d^3\boldsymbol{r}\hat{\rho}(\boldsymbol{r})$. This ensures that $\hat{\rho}(\boldsymbol{q})$ has the dimension of density (which it doesn't if we use $\sqrt{V}$ factors as in the canonical normalisation introduced in the lectures.)

b) Show that $<\hat{\rho}(\boldsymbol{q})> = n_0\delta_{\boldsymbol{q},0}$. (Remember we are using $\hat{\rho}(\boldsymbol{q}) = \frac{1}{V}\sum_{\boldsymbol{k}} \hat{c}^\dagger_{\boldsymbol{k}+\boldsymbol{q}}\hat{c}_{\boldsymbol{k}}$.)

c) Approximate

$$\hat{\rho}(\boldsymbol{q})\hat{\rho}(-\boldsymbol{q}) \quad \text{by} \quad <\hat{\rho}(\boldsymbol{q})>\hat{\rho}(-\boldsymbol{q}) + \hat{\rho}(\boldsymbol{q})<\hat{\rho}(-\boldsymbol{q})> - <\hat{\rho}(\boldsymbol{q})><\hat{\rho}(-\boldsymbol{q})>.$$

This is a mean-field approximation called the Hartree approximation. Which term has been neglected in making this substitution?

d) Explain why the Hamiltonian for the homogeneous electron gas in the Hartree approximation reduces to

$$\hat{H}_{\text{Har}} = \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}} \hat{c}^{\dagger}_{\boldsymbol{k},\sigma} \hat{c}_{\boldsymbol{k},\sigma},$$

ie the Hartree approximation is what you have been using all along when discussing free electrons.

a) n_0 is the density of the system. If the system is neutral the postive background density must equal the density of electrons.

b) The point here is that the operator $\hat{c}^{\dagger}(\boldsymbol{k}+\boldsymbol{q})\hat{c}(\boldsymbol{k})$, which appears in the density operator, only has a non-zero expectation value if $q = 0$ and $k < k_F$. So

$$\langle \hat{\rho}(\boldsymbol{q}) \rangle = \frac{1}{V} \sum_{\boldsymbol{k}} \langle \hat{c}^{\dagger}(\boldsymbol{k}+\boldsymbol{q})\hat{c}(\boldsymbol{k}) \rangle = \delta_{q,0} \frac{1}{V} \sum_{\boldsymbol{k}} \langle \hat{n}(\boldsymbol{k}) \rangle = n_0 \delta_{q,0}$$

c) We have dropped the term describing interactions between fluctuations about the mean field values:

$$(\hat{\rho}(\boldsymbol{q}) - <\hat{\rho}(\boldsymbol{q})>)(\hat{\rho}(-\boldsymbol{q}) - <\hat{\rho}(-\boldsymbol{q})>)$$

Check in the section on mean field theories in the lecture notes for more on this. There, we were looking at another mean field but the principle remains the same.

d) We insert the result from part b) into part c). This leaves only the terms involving $\hat{\rho}(0)$. These are cancelled by the interaction with the background charge.

12. (**) This question asks you to work through the Hartree-Fock approximation. This describes the Hartree approximation with an added expectation value affecting only particles with the same spin.

The interaction between like spins, $V_\sigma = \frac{1}{2}\sum_{\boldsymbol{q}} v(q)\hat{\rho}_\sigma(\boldsymbol{q})\hat{\rho}_\sigma(-\boldsymbol{q})$, can be written

$$\begin{aligned} V_\sigma &= \frac{1}{2V^2} \sum_{\boldsymbol{q}} v(q) \sum_{\boldsymbol{k}} \sum_{\boldsymbol{k}'} \hat{c}^{\dagger}_{\boldsymbol{k}+\boldsymbol{q},\sigma} \hat{c}_{\boldsymbol{k},\sigma} \hat{c}^{\dagger}_{\boldsymbol{k}'-\boldsymbol{q},\sigma} \hat{c}_{\boldsymbol{k}',\sigma} \\ &= -\frac{1}{2}\frac{1}{V^2} \sum_{\boldsymbol{q}} v(q) \sum_{\boldsymbol{k}} \sum_{\boldsymbol{k}'} \left(\hat{c}^{\dagger}_{\boldsymbol{k}+\boldsymbol{q},\sigma} \hat{c}_{\boldsymbol{k}',\sigma} \hat{c}^{\dagger}_{\boldsymbol{k}'-\boldsymbol{q},\sigma} \hat{c}_{\boldsymbol{k},\sigma} - \hat{c}^{\dagger}_{\boldsymbol{k}+\boldsymbol{q},\sigma} \hat{c}_{\boldsymbol{k},\sigma} \delta_{\boldsymbol{k}'-\boldsymbol{q},\boldsymbol{k}'} - \hat{c}^{\dagger}_{\boldsymbol{k}+\boldsymbol{q},\sigma} \hat{c}_{\boldsymbol{k}',\sigma} \delta_{\boldsymbol{k}'-\boldsymbol{q},\boldsymbol{k}} \right) \\ &= -\frac{1}{2}\frac{1}{V^2} \sum_{\boldsymbol{q}} v(q) \sum_{\boldsymbol{k}} \sum_{\boldsymbol{k}'} \hat{c}^{\dagger}_{\boldsymbol{k}+\boldsymbol{q},\sigma} \hat{c}_{\boldsymbol{k}',\sigma} \hat{c}^{\dagger}_{\boldsymbol{k}'-\boldsymbol{q},\sigma} \hat{c}_{\boldsymbol{k},\sigma} + \frac{1}{2}\frac{1}{V^2} \sum_{\boldsymbol{k}} \sum_{\boldsymbol{k}'} \left(v(0) + v(|\boldsymbol{k}-\boldsymbol{k}'|) \right) \hat{c}^{\dagger}_{\boldsymbol{k},\sigma} \hat{c}_{\boldsymbol{k},\sigma}. \end{aligned}$$

After the summation over $\boldsymbol{k}'$ the second term on the right hand side is a constant which we will drop for now. Now approximate the remaining term:

$$\begin{aligned} V_\sigma \approx -\frac{1}{2}\frac{1}{V^2} \sum_{\boldsymbol{q}} v(q) \sum_{\boldsymbol{k}} \sum_{\boldsymbol{k}'} \Big(&<\hat{c}^{\dagger}_{\boldsymbol{k}+\boldsymbol{q},\sigma} \hat{c}_{\boldsymbol{k}',\sigma}> \hat{c}^{\dagger}_{\boldsymbol{k}'-\boldsymbol{q},\sigma} \hat{c}_{\boldsymbol{k},\sigma} + \hat{c}^{\dagger}_{\boldsymbol{k}+\boldsymbol{q},\sigma} \hat{c}_{\boldsymbol{k}',\sigma} <\hat{c}^{\dagger}_{\boldsymbol{k}'-\boldsymbol{q},\sigma} \hat{c}_{\boldsymbol{k},\sigma}> \\ &- <\hat{c}^{\dagger}_{\boldsymbol{k}+\boldsymbol{q},\sigma} \hat{c}_{\boldsymbol{k}',\sigma}><\hat{c}^{\dagger}_{\boldsymbol{k}'-\boldsymbol{q},\sigma} \hat{c}_{\boldsymbol{k},\sigma}> \Big) \end{aligned}$$

(a) Explain why

$$<\hat{c}^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma}\hat{c}_{\boldsymbol{k}',\sigma}>=\delta_{\boldsymbol{k}+\boldsymbol{q},\boldsymbol{k}'}\theta(k_F-k') \quad \text{and} \quad <\hat{c}^\dagger_{\boldsymbol{k}'-\boldsymbol{q},\sigma}\hat{c}_{\boldsymbol{k},\sigma}>=\delta_{\boldsymbol{k}'-\boldsymbol{q},\boldsymbol{k}}\theta(k_F-k).$$

Here the expectation value is with respect to the filled Fermi sea, $|\psi_0\rangle = \prod_{k<k_F}(\hat{c}^\dagger_{\boldsymbol{k},\uparrow}\hat{c}^\dagger_{\boldsymbol{k},\downarrow})|0\rangle$, and θ is the Heaviside function.

(b) Show that the two non-constant terms give

$$V_\sigma \approx -\frac{1}{V}\sum_{\boldsymbol{k}}\left(\frac{1}{V}\sum_{\boldsymbol{k}'} v(|\boldsymbol{k}-\boldsymbol{k}'|)\theta(k_F-k')\right)\hat{c}^\dagger_{\boldsymbol{k},\sigma}\hat{c}_{\boldsymbol{k},\sigma}.$$

(c) The potential in the previous part is called the exchange potential. This is because it comes from matrix elements between components in a single Slater determinant with particles i and j switched round (or exchanged). You can evaluate it as follows. Replace the sum over $\boldsymbol{k}'$ by an integral and substitute for $v(q) = e^2/|\boldsymbol{k}-\boldsymbol{k}'|^2$.

$$V_{ex}(k) = -\frac{1}{V}\sum_{\boldsymbol{k}'} v(|\boldsymbol{k}-\boldsymbol{k}'|)\theta(k_F-k') \to \int_{k'<k_F}\frac{d^3\boldsymbol{k}'}{(2\pi)^3}\frac{e^2}{|\boldsymbol{k}-\boldsymbol{k}'|^2}$$

Unless you like doing integrals you can skip this part but you should note the answer. To do the integrals take the origin at $k'=0$, choose the z-axis parallel to $\boldsymbol{k}$ so that $|\boldsymbol{k}-\boldsymbol{k}'|^2 = k'^2+k^2-2k'k\cos\theta_{k'}$. You should find

$$V_\sigma = -\frac{e^2k_F}{2\pi^2}\left(\frac{1}{2}+\frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right|\right),$$

where $x = k/k_F$.

(d) The answer in part c) should cause you to raise your eyebrows a little as it appears to have non-analytic behaviour at $x=1$, *ie* at the Fermi energy. This leads to a strange prediction. If you combine the result for V_σ with the kinetic energy, you obtain

$$\hat{H} = \sum_{\boldsymbol{k},\sigma}(\epsilon_{\boldsymbol{k}}+V_\sigma(x))\hat{c}^\dagger_{\boldsymbol{k},\sigma}\hat{c}_{\boldsymbol{k},\sigma} \equiv \sum_{\boldsymbol{k},\sigma}\tilde{\epsilon}_{\boldsymbol{k}}\hat{c}^\dagger_{\boldsymbol{k},\sigma}\hat{c}_{\boldsymbol{k},\sigma}.$$

The energy of the plane wave state is now $\tilde{\epsilon}_k$. Write

$$V_\sigma = -\frac{e^2k_F}{2\pi^2}F(x),$$

and compute F'(x). What happens at $x=1$ and what does this say about the nature of the system? Remember that the density of states in energy varies as

$$k^2dk \sim E\frac{dk}{dE}dE.$$

a) The state, $\hat{c}_{\boldsymbol{k}',\sigma}|FS\rangle = 0$, unless $k' < k_F$. Similarly, $\langle FS|\hat{c}^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma} = 0$, unless $|\boldsymbol{k}+\boldsymbol{q}| < k_F$.

b) Insert the result from (a) into the expression for V_σ to find the result.

c) Write out the integral in the variables suggested

$$\begin{aligned}
V_{ex}(k) &= \frac{e^2}{(2\pi)^2}\int_0^{k_F} dk' \int_0^{\pi} d\theta_{k'} \frac{k'^2 \sin\theta_{k'}}{k^2 + k'^2 - 2kk'\cos\theta_{k'}} \\
&= \frac{e^2}{(2\pi)^2}\int_0^{k_F} dk'\, k'^2 \left[\frac{1}{2kk'}\ln(k^2 + k'^2 - 2kk'\cos\theta_{k'})\right]_0^{\pi} \\
&= \frac{e^2}{(2\pi)^2}\int_0^{k_F} dk' \frac{k'}{k}\ln\left|\frac{k+k'}{k-k'}\right|
\end{aligned}$$

For the second integral, write $y = k'/k$ and $x = k/k_F$

$$\begin{aligned}
V_{ex}(k) &= -\frac{e^2 k}{(2\pi)^2}\int_0^{k_F/k} dy\, y \ln\left|\frac{1+y}{1-y}\right| \\
&= -\frac{e^2 k}{(2\pi)^2}\left(\left[\frac{y^2}{2}\ln\left|\frac{1+y}{1-y}\right|\right]_0^{k_F/k} - \int_0^{k_F/k} dy\, \frac{y^2}{2}\left(\frac{1}{1+y} + \frac{1}{1-y}\right)\right) \\
&= -\frac{e^2 k_F}{(2\pi)^2} x\left(\frac{1}{2x^2}\ln\left|\frac{1+x}{1-x}\right| - \int_0^{k_F/k} dy\, \frac{y}{2}\left(\frac{1+y-1}{1+y} - \frac{1-y-1}{1-y}\right)\right) \\
&= -\frac{e^2 k_F}{(2\pi)^2} x\left(\frac{1}{2x^2}\ln\left|\frac{1+x}{1-x}\right| - \int_0^{k_F/k} dy\, \frac{y}{2}\left(\frac{-1}{1+y} + \frac{1}{1-y}\right)\right) \\
&= -\frac{e^2 k_F}{(2\pi)^2} x\left(\frac{1}{2x^2}\ln\left|\frac{1+x}{1-x}\right| - \int_0^{k_F/k} dy\, \frac{1}{2}\left(\frac{-1-y+1}{1+y} + \frac{y-1+1}{1-y}\right)\right) \\
&= -\frac{e^2 k_F}{(2\pi)^2} x\left(\frac{1}{2x^2}\ln\left|\frac{1+x}{1-x}\right| - \int_0^{k_F/k} dy\, \frac{1}{2}\left(-2 + \frac{1}{1+y} + \frac{1}{1-y}\right)\right) \\
&= -\frac{e^2 k_F}{(2\pi)^2} x\left(\frac{1}{2x^2}\ln\left|\frac{1+x}{1-x}\right| + \frac{1}{x} - \frac{1}{2}\ln\left|\frac{1+x}{1-x}\right|\right) \\
&= -\frac{e^2 k_F}{2\pi^2}\left(\frac{1}{2} + \frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right|\right).
\end{aligned}$$

d) Differentiating wrt x and putting $x = 1 + \epsilon$ gives

$$\begin{aligned}
F'(x) &\sim \left(-\frac{1}{x^2} - 1\right)\ln\left|\frac{1+x}{1-x}\right| + \left(\frac{1}{x} - x\right)\left(\frac{1}{1+x} + \frac{1}{1-x}\right) \\
&\approx -2(\ln 2 - \ln|\epsilon|) + 2.
\end{aligned}$$

In the limit $\epsilon \to 0$, $F'(x) \to \infty$. This means $d\tilde{\epsilon}_k/dk \to \infty$ and $dk/dE \to 0$ implying vanishing density of states. Consequently the system described by HF is not a metal.

The Hartree-Fock theory has virtues but is often not a good theory on its own (as we see here for the homogeneous electron gas). As well as a vanishing density of states at the Fermi energy it greatly overestimates the bandwidth for excitations in materials. To do better would require including what are called correlation effects. These are defined as effects where the state of a particle is correlated with the motion of other individual particles and not just with their average value (as in the Hartree or Hartree-Fock approximation).

The origin of the non-analytic behaviour is the discontinuity in the occupation of states at the Fermi energy. If a discontinuity of this type continues to exist even after treating correlation effects, the system is called a Fermi liquid. It also has consequences in response functions—look up Friedel oscillations for an example.

Spin Waves

(We did not cover this material in lectures, but feel free to read chapter 4 and have a go.)

13. When discussing the Heisenberg Hamiltonian for an antiferromagnet we introduced the canonical transformation:

$$\begin{pmatrix} \hat{\alpha}_{\boldsymbol{q}} \\ \hat{\beta}^\dagger_{\boldsymbol{q}} \end{pmatrix} = \begin{pmatrix} \cosh\theta_{\boldsymbol{q}} & \sinh\theta_{\boldsymbol{q}} \\ \sinh\theta_{\boldsymbol{q}} & \cosh\theta_{\boldsymbol{q}} \end{pmatrix} \begin{pmatrix} \hat{a}_{\boldsymbol{q}} \\ \hat{b}^\dagger_{-\boldsymbol{q}} \end{pmatrix},$$

(a) We can write this in the form

$$\hat{\alpha}_{\boldsymbol{q}} = U\hat{a}_{\boldsymbol{q}}U^{-1} \quad \text{and} \quad \hat{\beta}^\dagger_{\boldsymbol{q}} = U\hat{b}^\dagger_{-\boldsymbol{q}}U^{-1} \quad \text{where} \quad U = e^{\theta_{\boldsymbol{q}}\left(\hat{a}^\dagger_{\boldsymbol{q}}\hat{b}^\dagger_{-\boldsymbol{q}} - \hat{b}_{-\boldsymbol{q}}\hat{a}_{\boldsymbol{q}}\right)}.$$

Verify this as follows. Consider the expressions for $\alpha_{\boldsymbol{q}}(\theta_{\boldsymbol{q}})$ and $\beta^\dagger_{\boldsymbol{q}}(\theta_{\boldsymbol{q}})$ involving U and find the equation

$$\frac{d}{d\theta_{\boldsymbol{q}}} \begin{pmatrix} \hat{\alpha}_{\boldsymbol{q}}(\theta_{\boldsymbol{q}}) \\ \hat{\beta}^\dagger_{\boldsymbol{q}}(\theta_{\boldsymbol{q}}) \end{pmatrix} = \theta_{\boldsymbol{q}}\sigma_x \begin{pmatrix} \hat{\alpha}_{\boldsymbol{q}}(\theta_{\boldsymbol{q}}) \\ \hat{\beta}^\dagger_{\boldsymbol{q}}(\theta_{\boldsymbol{q}}) \end{pmatrix},$$

where σ_x is the Pauli matrix. This equation should integrate to give the required result.

(b) This transformation also acts on states. The canonical transformation takes the form

$$|0\rangle \to |0'\rangle = U|0\rangle$$

where $|0\rangle$ is the vacuum containing no $\hat{a}$ bosons. Verify that

$$\hat{\alpha}_{\boldsymbol{q}}|0'\rangle = 0 \quad \text{and} \quad \hat{\beta}_{\boldsymbol{q}}|0'\rangle = 0$$

(Note: $|0'\rangle$ is the ground state of the system with Hamiltonian $\sim \sum_{\boldsymbol{q}} \epsilon_{\boldsymbol{q}}(\hat{\alpha}^\dagger_{\boldsymbol{q}}\hat{\alpha}_{\boldsymbol{q}} + \hat{\beta}^\dagger_{\boldsymbol{q}}\hat{\beta}_{\boldsymbol{q}})$.)

(a) Find

$$\begin{aligned} \frac{d}{d\theta_{\boldsymbol{q}}} \begin{pmatrix} \hat{\alpha}_{\boldsymbol{q}}(\theta_{\boldsymbol{q}}) \\ \hat{\beta}^\dagger_{\boldsymbol{q}}(\theta_{\boldsymbol{q}}) \end{pmatrix} &= \theta_{\boldsymbol{q}} \begin{pmatrix} U\left[\left(\hat{a}^\dagger_{\boldsymbol{q}}\hat{b}^\dagger_{-\boldsymbol{q}} - \hat{b}_{-\boldsymbol{q}}\hat{a}_{\boldsymbol{q}}\right), \hat{a}_{\boldsymbol{q}}\right]U^{-1} \\ U\left[\left(\hat{a}^\dagger_{\boldsymbol{q}}\hat{b}^\dagger_{-\boldsymbol{q}} - \hat{b}_{-\boldsymbol{q}}\hat{a}_{\boldsymbol{q}}\right), \hat{b}^\dagger_{-\boldsymbol{q}}\right]U^{-1} \end{pmatrix} \\ &= \theta_{\boldsymbol{q}} \begin{pmatrix} U(-\hat{b}^\dagger_{-\boldsymbol{q}})U^{-1} \\ U(-\hat{a}_{\boldsymbol{q}})U^{-1} \end{pmatrix} = -\theta_{\boldsymbol{q}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \hat{\alpha}_{\boldsymbol{q}} \\ \hat{\beta}^\dagger_{\boldsymbol{q}} \end{pmatrix} \end{aligned}$$

Hence identify σ_x. Integrating formally gives (I is the identity matrix)

$$\begin{aligned} \begin{pmatrix} \hat{\alpha}_{\boldsymbol{q}}(\theta_{\boldsymbol{q}}) \\ \hat{\beta}^\dagger_{\boldsymbol{q}}(\theta_{\boldsymbol{q}}) \end{pmatrix} &= \mathrm{e}^{-\theta_{\boldsymbol{q}}\,\sigma_x} \begin{pmatrix} \hat{\alpha}_{\boldsymbol{q}}(0) \\ \hat{\beta}^\dagger_{-\boldsymbol{q}}(0) \end{pmatrix} = \mathrm{e}^{-\theta_{\boldsymbol{q}}\,\sigma_x} \begin{pmatrix} \hat{a}_{\boldsymbol{q}} \\ \hat{b}^\dagger_{-\boldsymbol{q}} \end{pmatrix} \\ &= \left(\left(1 + \frac{\theta_{\boldsymbol{q}}^2}{2} + \frac{\theta_{\boldsymbol{q}}^4}{4!} + \ldots\right) I - \left(\theta_{\boldsymbol{q}}^2 + \frac{\theta_{\boldsymbol{q}}^3}{3!} + \ldots\right)\sigma_x\right) \begin{pmatrix} \hat{a}_{\boldsymbol{q}} \\ \hat{b}^\dagger_{-\boldsymbol{q}} \end{pmatrix} \\ &= \begin{pmatrix} \cosh\theta_{\boldsymbol{q}} & -\sinh\theta_{\boldsymbol{q}} \\ -\sinh\theta_{\boldsymbol{q}} & \cosh\theta_{\boldsymbol{q}} \end{pmatrix} \begin{pmatrix} \hat{a}_{\boldsymbol{q}} \\ \hat{b}^\dagger_{-\boldsymbol{q}} \end{pmatrix}. \end{aligned}$$

(b) Insert for $\hat{\alpha}_{\boldsymbol{q}}$ and $|0'\rangle$:

$$\hat{\alpha}_{\boldsymbol{q}}|0'\rangle = U\hat{a}_{\boldsymbol{q}}U^{-1}U|0\rangle = U\hat{a}_{\boldsymbol{q}}|0\rangle = 0$$

Density Matrix

14. Let $|\uparrow\rangle$ and $|\downarrow\rangle$ label the basis states of a spin-1/2 particle. Here $|\uparrow\rangle$ has $\sigma_z = 1$. Consider a state

$$|\psi\rangle = \frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}}.$$

Compute the density matrix, $\hat{\rho}$ (see section 5.1 to find how the density matrix for a system described by a wavefunction is defined).

(a) Verify that $\hat{\rho}^2 = 1$. Is this a pure or a mixed state?

(b) Using the density matrix compute the average values $< \sigma^z >$ and $< \sigma^x >$.

(c) Now consider a density matrix describing a system with equal probability that $\sigma^z = 1$ and that $\sigma^z = -1$. Compute $\hat{\rho}^2 = 1$ for this density matrix. Assume equal probabilities for the two basis states. Is this a pure or a mixed state?

(d) Compute $< \sigma^x >$ for the system described by the density matrix in part c). Comment on the difference to the result you found in part a).

(a)

$$\hat{\rho} = |\psi\rangle\langle\psi| \quad \Rightarrow \quad \hat{\rho}^2 = |\psi\rangle\langle\psi||\psi\rangle\langle\psi| = \hat{\rho}.$$

(b) Write $\hat{\rho} = |i\rangle\rho_{ij}\langle j|$ with

$$\rho_{ij} = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}.$$

This gives

$$< \sigma^z > = \mathrm{Tr}\,\rho\,\sigma^z = \mathrm{Tr} \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1/2 & 1/2 \\ -1/2 & -1/2 \end{pmatrix} = 0$$

$$< \sigma^x > = \mathrm{Tr}\,\rho\,\sigma^x = \mathrm{Tr} \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} = 1.$$

(c) Now

$$\rho_{ij} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \quad \text{and} \quad \rho_{ij}^2 = \begin{pmatrix} 1/4 & 0 \\ 0 & 1/4 \end{pmatrix}.$$

This is a mixed state $\mathrm{Tr}\,\rho^2 = 1/2 < 1$.

(d) For this state

$$< \sigma^x > = \mathrm{Tr}\,\rho\,\sigma^x = \mathrm{Tr} \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1/2 \\ 1/2 & 0 \end{pmatrix} = 0.$$

All we know is that the state has equal probability to be in the up and the down states. If the state were to have non-zero $< \sigma^x >$, or $< \sigma^y >$, we would need more information. This is to be expected for a mixed state - the system is not in a single wavefunction.