Condensed Matter Theory

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Abstract: Lecture notes for the course Condensed Matter Theory 1, taught by Brian M. Andersen.

Contents

1 Second Quantization

1.1 1D Chain

We begin with a classical 1D discrete chain

$$H = \sum_{j=1}^{N} \left(\frac{\pi_j^2}{2m} + \frac{m\omega^2}{2} (\phi_j - \phi_{j+1})^2 \right) , \tag{1.1}$$

with ϕ_j being the displacement and π_j the momentum of the chain in the j-th site, N the total number of sites. If the spacing between the sites is a, the Fourier components of π_j and ϕ_j can be written as

$$\phi_j = \frac{1}{\sqrt{N}} \sum_q \phi_q e^{iqaj} , \qquad \pi_j = \frac{1}{\sqrt{N}} \sum_q \pi_q e^{iqaj} . \tag{1.2}$$

Imposing periodic boundary conditions means that $\phi_{N+1} = \phi_1$, so

$$e^{iqNa} = 1 \qquad \to \qquad q = \frac{2\pi}{Na} n , \text{ with}\, n \in \mathbb{Z} . \tag{1.3}$$

In the kinetic term we get

$$\begin{aligned} \sum_{j=1}^{N} \left(\frac{\pi_j^2}{2m} \right) &= \frac{1}{2mN} \sum_{j=1}^{N} \sum_{q,q'} (\pi_q e^{iqaj})(\pi_{q'} e^{iq'aj}) \\ &= \frac{1}{2m} \sum_{q,q'} \pi_q \pi_{q'} \underbrace{\left(\frac{1}{N} \sum_{j=1}^{N} e^{i(q+q')aj} \right)}_{\delta_{q,-q'}} \\ &= \frac{1}{2m} \sum_q \pi_q \pi_{-q} \end{aligned} \tag{1.4}$$

and doing the same for the potential energy we get the Hamiltonian

$$H = \sum_q \left(\frac{1}{2m} \pi_q \pi_{-q} + \frac{m\omega_q}{2} \phi_q \phi_{-q} \right) , \qquad \omega_q = 2\omega \left| sin \left(\frac{qa}{2} \right) \right| \tag{1.5}$$

We now procede with a canonical quantization of the conjugate variables

$$\left[\phi_q, \pi_{q'} \right] = i\hbar \delta_{q,q'} , \tag{1.6}$$

$$\phi_q = \sqrt{\frac{\hbar}{2m\omega_q}} \left(a_q + a_{-q}^\dagger \right) , \qquad \pi_q = -i \sqrt{\frac{\hbar m\omega_q}{2}} \left(a_q - a_{-q}^\dagger \right) \tag{1.7}$$

$$\to \left[a_q, a_{q'}^\dagger \right] = \delta_{q,q'} \tag{1.8}$$

so $a_q, a_q^\dagger$ are the annihilation/creation operators for the mode q. The Hamiltonian, now diagonalized, becomes

$$H = \sum_q \hbar\omega_q \left(a_q a_q^\dagger + \frac{1}{2} \right) \tag{1.9}$$

Now, the next one is the most important step of all: instead of giving ϕ_j, π_j for every site, we describe the *many-body* system by saying how many excitations n_q there are in every mode q

$$|\Psi\rangle = |n_1, n_2, ..., n_N\rangle = \prod_{q=1}^{N} \frac{(a_q^\dagger)^{n_q}}{\sqrt{n_q}} |0\rangle \tag{1.10}$$

with $|0\rangle$ vacuum state. That's what we will try to do now on for every many-body system we encounter.

1.2 New operators

The second most important step is to promote the wave function to an operator field

$$\psi(x) \qquad \rightarrow \qquad \hat{\psi}(x) \tag{1.11}$$

In standard QM the expectation values of (hermitian) operators can be seen as a functional $O[\psi, \psi^*]$, so we also promote them to operators $\hat{O}$ (think that functionals are just the simplest case of operators). For example, the kinetic energy becomes

$$T = \int d^3x\, \psi^*(x) \left(-\frac{\hbar^2}{2m} \nabla_x^2 \right) \psi(x) \quad \rightarrow \quad \hat{T} = \int d^3x \int d^3y\, \hat{\psi}^\dagger(x) \left(-\frac{\hbar^2}{2m} \nabla_x^2 \right) \delta(x-y) \hat{\psi}(y). \tag{1.12}$$

Notice that we have two kinds of operators: field operators and observable operators Why does it make sense to turn the wave function into an operator? Let's take a state $|\psi(t)\rangle$ in Hilbert space and a complete set $\{|m\rangle\}$, such that $\sum_m |m\rangle \langle m| = \mathbb{1}$. We can expand the state onto this basis

$$|\psi(t)\rangle = \sum_m |m\rangle\langle m|\psi(t)\rangle \tag{1.13}$$

Using Schröedinger's equation and projecting onto a state $|n\rangle$ we get

$$\langle n|i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \langle n|H|m\rangle = \sum_m \langle n|H|m\rangle\langle m|\psi(t)\rangle \tag{1.14}$$

$$\begin{aligned} i\hbar\dot{\psi}_n(t) &= \sum_m H_{nm}\psi_m(t) \\ i\hbar\dot{\psi}_n^*(t) &= -\sum_m H_{mn}\psi_m^*(t)\ (c.c.) \end{aligned} \tag{1.15}$$

To finsh off, let's look at the expectation value of the Hamiltonian

$$\langle H\rangle = \langle\psi(t)|H|\psi(t)\rangle = \sum_m \sum_n H_{nm}\psi_m^*(t)\psi_n(t) \tag{1.16}$$

$$\rightarrow \begin{cases} \dot{\psi}_n = \frac{\partial}{\partial(i\hbar\psi_n)} \langle H\rangle \\ i\hbar\dot{\psi}_n^* = -\frac{\partial}{\partial\psi_n} \langle H\rangle \end{cases} \tag{1.17}$$

Notice that they look exactly like Hamilton's equations for Classical Mechanics, this means that $(\psi_n\,, i\hbar\psi_m^*)$ are canonically conjugate variables. In analogy with what we did in standard QM with position and momentum $(q\,, p)$, we can promote these variables to operators and impose the commutation relations

$$\left[\hat{\psi}_n, \hat{\psi}_m\right]_\pm = \left[\hat{\psi}_n^\dagger, \hat{\psi}_m^\dagger\right]_\pm = 0\,, \tag{1.18}$$

$$\left[\hat{\psi}_n, \hat{\psi}_m^\dagger\right]_\pm = \delta_{nm}\,. \tag{1.19}$$

This commutation/anti-commutation algebra leads to the properties of bosons (harmonic oscillator) for the minus sign or fermions for the plus sign.

1.3 Whatever basis

Let's start in the most general case, later we will see special cases where the basis sets are eingestates of the position operator, or the momentum operator, or the Hamiltonian. For two complete sets $\{|n\rangle\}$, $\{|\tilde{m}\rangle\}$

$$\begin{aligned} |\Psi\rangle &= \sum\!\!\!\!\!\!\!\int_n |n\rangle\langle n|\Psi\rangle = \sum\!\!\!\!\!\!\!\int_{\tilde{m}} |\tilde{m}\rangle\langle\tilde{m}|\Psi\rangle \\ &= \sum\!\!\!\!\!\!\!\int_n \psi_n|n\rangle = \sum\!\!\!\!\!\!\!\int_{\tilde{m}} \phi_{\tilde{m}}|\tilde{m}\rangle \end{aligned} \tag{1.20}$$

where the symbol $\sum\!\!\!\!\!\!\int$ is used meaning that the sets could be either discrete or continuous, leading to ψ and ϕ being either discrete coefficients or functions. Projecting onto an element of the "tilda" basis we get

$$\phi_{\tilde{m}} = \langle\tilde{m}|\Psi\rangle = \sum\!\!\!\!\!\!\!\int_n \langle\tilde{m}|n\rangle\,\psi_n \xrightarrow[2^{nd}\text{ quant.}]{} \hat{\phi}_{\tilde{m}} = \sum\!\!\!\!\!\!\!\int_n \langle\tilde{m}|n\rangle\,\hat{\psi}_n \tag{1.21}$$

which is the rule for how field operators transform. Notice how in the case of position and momentum basis, since $\langle x|k\rangle \propto e^{ikx}$, we get the definition of the Fourier transform of field operators. If the complete sets we are switching through are orthonormal then the commutation realations are conserved

$$[\hat{\phi}_{\tilde{l}}, \hat{\phi}_{\tilde{m}}^\dagger]_\pm = \sum\!\!\!\!\!\!\!\int_{n,p} \langle\tilde{l}|n\rangle\langle p|\tilde{m}\rangle\,\underbrace{[\hat{\psi}_n, \hat{\psi}_p^\dagger]_\pm}_{\delta_{np}} = \langle\tilde{l}|\underbrace{\left(\sum\!\!\!\!\!\!\!\int_n |n\rangle\langle n|\right)}_{\mathbb{1}}|\tilde{m}\rangle = \delta_{\tilde{l}\tilde{m}} \tag{1.22}$$

1.4 Position eigenstates basis

The ladder operators can create states from the vacuum in different basis. In real space for example they can be used to create eigenstates of position

$$\hat{\psi}^\dagger(x)|0\rangle = |x\rangle$$

From the continuous orthonormality relation we get

$$\delta(x - x') = \langle x|x'\rangle = \langle 0|\hat{\psi}(x)\hat{\psi}^\dagger(x')|0\rangle \tag{1.23}$$

and since the effect of the lowering operator is $\hat{\psi}(x)|0\rangle = 0$, we can insert the commuted term and get the commutator inside

$$\delta(x-x') = \langle 0|[\hat{\psi}(x)\,,\hat{\psi}^\dagger(x')]_\pm|0\rangle \tag{1.24}$$

which of course it's just the continuous version of 1.19.

We can create multiple eigenstates of position

$$|x_1,...,x_N\rangle = \hat{\psi}^\dagger(x_N)...\hat{\psi}^\dagger(x_1)|0\rangle \tag{1.25}$$

which can then be used to write the good old wavefunction for a many-body state $|\Psi\rangle$

$$\begin{aligned}\Psi(x_1,...,x_N) &= \langle x1,...,x_N|\Psi\rangle \\ &= \langle 0|\hat{\psi}(x_1)...\hat{\psi}(x_N)|\Psi\rangle\end{aligned} \tag{1.26}$$

1.5 Energy eigenstates basis

If $\{|n\rangle\}$ are the eigenstates of $\hat{H}$, then they form a complete set because of the spectral theorem ($\hat{H}$ is an observable so it's hermitian). In its eigenstates basis $\hat{H}$ is diagonal

$$\langle n|\hat{H}|m\rangle = E_m\delta_{nm}\,, \qquad \hat{H} = \sum_{nm}\hat{\psi}_n^\dagger E_m\delta_{nm}\hat{\psi}_m = \sum_n E_n\hat{\psi}_n^\dagger\hat{\psi}_n\,. \tag{1.27}$$

For example in real space we would get

$$\begin{aligned}\hat{H} &= \sum_n E_n \underbrace{\int d^3x\langle x|n\rangle\hat{\psi}^\dagger(x)}_{\hat{\psi}_n^\dagger}\underbrace{\int d^3y\langle n|y\rangle\hat{\psi}(y)}_{\hat{\psi}_n} \\ &= \sum_{nm} E_m\delta_{nm}\int d^3x\langle x|n\rangle\hat{\psi}^\dagger(x)\int d^3y\langle m|y\rangle\hat{\psi}(y) \\ &= \sum_{nm}\langle n|\hat{H}|m\rangle\int d^3x\langle x|n\rangle\hat{\psi}^\dagger(x)\int d^3y\langle m|y\rangle\hat{\psi}(y) \\ &= \int d^3x\int d^3y\sum_{nm}\langle x|n\rangle\langle n|\hat{H}|m\rangle\langle m|y\rangle\hat{\psi}^\dagger(x)\hat{\psi}(y) \\ &= \int d^3x\int d^3y\langle x|\left(\sum_n|n\rangle\langle n|\right)\hat{H}\left(\sum_m|m\rangle\langle m|\right)|y\rangle\hat{\psi}^\dagger(x)\hat{\psi}(y) \\ &= \int d^3x\int d^3y\langle x|\hat{H}|y\rangle\hat{\psi}^\dagger(x)\hat{\psi}(y)\,.\end{aligned} \tag{1.28}$$

For a free hamiltonian we have $\langle x|\hat{H}|y\rangle = -\frac{\hbar^2}{2m}\nabla_x^2\,\delta(x-y)$, so

$$\hat{H}^0 = \int d^3x\,\hat{\psi}^\dagger(x)\left(-\frac{\hbar^2}{2m}\nabla_x^2\right)\hat{\psi}(x) \tag{1.29}$$

which is what we said at the beginning of the chapter about promoting QM's expectation values to operators.

1.6 Momentum eigenstates basis

When a system has translational invariance it is useful to use the eigenstates of momentum as a basis, since the momentum is the generator of space translations. The particle annihilation operator is

$$\hat{\psi}(x) = \sum_q \langle x|q\rangle \, \hat{c}_q = \frac{1}{\sqrt{V}} \sum_q e^{iqx} \hat{c}_q$$

The free Hamiltonian then is

$$\begin{aligned}
\hat{H}^0 &= -\frac{\hbar^2}{2m} \int d^3x \hat{\psi}^\dagger(x) \, \nabla_x^2 \, \hat{\psi}(x) \\
&= -\frac{\hbar^2}{2mV} \int d^3x \sum_{q,q'} e^{-iqx} \, \hat{c}_q^\dagger \, (iq')^2 \, e^{iq'x} \, \hat{c}_{q'} \\
&= \frac{\hbar^2}{2m} \sum_{q,q'} (q')^2 \, \hat{c}_q^\dagger \hat{c}_{q'} \, \underbrace{\frac{1}{V} \int d^3x \, e^{i(q'-q)x}}_{\delta_{q',q}} \\
&= \sum_q \frac{\hbar^2 q^2}{2m} \hat{c}_q^\dagger \hat{c}_{q'}
\end{aligned}$$

A two particle state for Fermions is naturally anti-symmetric

$$|\Psi\rangle = |k_1, k_2\rangle = \hat{c}_{k_2}^\dagger \hat{c}_{k_1}^\dagger |0\rangle$$

$$\begin{aligned}
\Psi(x_1, x_2) &= \langle x_1, x_2|\Psi\rangle = \langle 0|\psi(x_1)\psi(x_2)\hat{c}_{k_2}^\dagger \hat{c}_{k_1}^\dagger|0\rangle \\
&= \langle 0|\psi(x_1)\psi(x_2) \int d^3x \langle x|k_2\rangle \hat{\psi}^\dagger(x) \int d^3y \langle y|k_1\rangle \hat{\psi}^\dagger(y)|0\rangle \\
&= \frac{1}{V} \int d^3x \int d^3y \, e^{ik_2x} e^{ik_1y} \, \langle 0|\psi(x_1)\psi(x_2)\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(y)|0\rangle \\
&= \frac{1}{V} \int d^3x \int d^3y \, e^{ik_2x} e^{ik_1y} \, \langle 0|\psi(x_1) \left[-\hat{\psi}^\dagger(x)\psi(x_2) + \delta(x_2 - x) \right] \hat{\psi}^\dagger(y)|0\rangle \\
&= \frac{1}{V} \int d^3x \int d^3y \, e^{ik_2x} e^{ik_1y} \, \langle 0| \left[-\psi(x_1)\hat{\psi}^\dagger(x)\delta(x_2 - y) + \psi(x_1)\hat{\psi}^\dagger(y)\delta(x_2 - x) \right] |0\rangle \\
&= \frac{1}{V} \int d^3x \int d^3y \, e^{ik_2x} e^{ik_1y} \, \left[\delta(x_1 - y)\delta(x_2 - x) - \delta(x_1 - x)\delta(x_2 - y) \right] \\
&= \frac{1}{V} \left(e^{ik_1x_1} e^{ik_2x_2} - e^{ik_1x_2} e^{ik_2x_1} \right)
\end{aligned}$$

1.7 Annihilation and creation operators

In analogy with what we did for the harmonic oscillator, we call the number operator $\hat{N} = \sum_n \hat{\psi}_n^\dagger \hat{\psi}_n$. There is a general property that relates commutators containing a product to either a sum of commutators or a difference of anti-commutator

$$[ab, c] = a[b, c]_\pm \mp [a, c]_\pm b \,. \tag{1.30}$$

For both bosons and fermions it then holds

$$[\hat{N},\hat{\psi}_n^\dagger] = \sum_l [\hat{\psi}_l^\dagger\hat{\psi}_l,\hat{\psi}_n^\dagger] = \sum_l \left(\hat{\psi}_l^\dagger \underbrace{[\hat{\psi}_l,\hat{\psi}_n^\dagger]_\pm}_{\delta_{ln}} \mp \cancel{[\hat{\psi}_l^\dagger,\hat{\psi}_n^\dagger]_\pm}\hat{\psi}_l \right) = \hat{\psi}_n^\dagger \tag{1.31}$$

$$[\hat{N},\hat{\psi}_n] = \sum_l [\hat{\psi}_l^\dagger\hat{\psi}_l,\hat{\psi}_n] = \sum_l \left(\hat{\psi}_l^\dagger \cancel{[\hat{\psi}_l,\hat{\psi}_n]_\pm} \mp \underbrace{[\hat{\psi}_l^\dagger,\hat{\psi}_n]_\pm}_{\pm\delta_{ln}}\hat{\psi}_l \right) = -\hat{\psi}_n \tag{1.32}$$

which is why we call them raising/lowering (in general ladder) operators

$$\hat{N}\hat{\psi}_n^\dagger = \hat{\psi}_n^\dagger(\hat{N}+1)\,, \qquad \hat{N}\hat{\psi}_n = \hat{\psi}_n(\hat{N}-1) \tag{1.33}$$

1.8 Differences between bosons and fermions

Bosons Up to now we only talked about them having the same properties, let's now talk about what's different between bosons and fermions. We already know the rules for bosons, since they're the same ones that (multiple) harmonic oscillators would have

$$[\hat{\psi}_i,\hat{\psi}_j^\dagger]_- = [\hat{\psi}_i,\hat{\psi}_j^\dagger] = \delta_{ij}\,, \qquad [\hat{\psi}_i^\dagger,\hat{\psi}_j^\dagger] = [\hat{\psi}_i,\hat{\psi}_j] = 0 \tag{1.34}$$

$$\hat{\psi}_i|0\rangle = 0\,, \qquad |n_1,...,n_N,...\rangle = \prod_{i=1}^{\infty} \frac{(\hat{\psi}_i^\dagger)^{n_i}}{\sqrt{n_i}}|0\rangle\,, \quad n_i \in \mathbb{N} \tag{1.35}$$

Notice that the many-body state being created is symmetric because $[\hat{\psi}_i^\dagger,\hat{\psi}_j^\dagger] = 0$.

Fermions For fermions the rules are different. The anti-commutation algebra is

$$[\hat{\psi}_i,\hat{\psi}_j^\dagger]_+ = \{\hat{\psi}_i,\hat{\psi}_j^\dagger\} = \delta_{ij}\,, \qquad \{\hat{\psi}_i^\dagger,\hat{\psi}_j^\dagger\} = \{\hat{\psi}_i,\hat{\psi}_j\} = 0 \tag{1.36}$$

So altough there is a vacuum state $\hat{\psi}_i|0\rangle = 0$, it is also true that

$$(\hat{\psi}_i)^2 = \frac{1}{2}\{\hat{\psi}_i,\hat{\psi}_j\} = 0\,, \qquad (\hat{\psi}_i^\dagger)^2 = \frac{1}{2}\{\hat{\psi}_i^\dagger,\hat{\psi}_j^\dagger\} = 0 \tag{1.37}$$

This means that we can raise only once a particle out of the vacuum, if we try to do it again we will get zero. Said in another way: contrary to the harmonic oscillator, here the ladder has only two steps. We have indeed already encountered this in QM, because ladder operators built out of Pauli matrices have the same anti-commuting algebra as fermionic field operators

$$\sigma_\pm = \frac{1}{\sqrt{2}}(\sigma_x \pm i\sigma_y) \tag{1.38}$$

$$\begin{aligned}\{\sigma_+,\sigma_-\} &= \frac{1}{2}\left[(\sigma_x+i\sigma_y)(\sigma_x-i\sigma_y)+(\sigma_x+i\sigma_y)(\sigma_x+i\sigma_y)\right]\\ &= \frac{1}{2}\left(\sigma_x^2 - i[\sigma_x,\sigma_y] + \sigma_y^2 + \sigma_x^2 + i[\sigma_x,\sigma_y] + \sigma_y^2\right) = 1.\end{aligned} \tag{1.39}$$

In that case the eingevalues of the z-component of spin were constrained between the two values $\pm 1/2$ (but it held in general for every angular momentum that $J_z = -J,...,+J$), wile in this case it is the occupation number that can only be 0 or 1.

A general fermionic state can then be written

$$|n_1, ..., n_N, ...\rangle = \prod_{i=1}^{\infty} (\hat{\psi}_i^\dagger)^{n_i} |0\rangle \,, \quad n_i \in \{0, 1\} \tag{1.40}$$

which is anti-symmetric because of the algebra $\{\hat{\psi}_i^\dagger, \hat{\psi}_j^\dagger\} = 0$. Given that there is an overall sign ambiguity, we stick to the convention that

$$\begin{aligned} \hat{\psi}_i^\dagger |n_1, ..., n_i, ...\rangle &= (-1)^{\Sigma_i} (1 - n_i) |n_1, ..., n_i + 1, ...\rangle \\ \hat{\psi}_i |n_1, ..., n_i, ...\rangle &= (-1)^{\Sigma_i} \, n_i \, |n_1, ..., n_i - 1, ...\rangle \end{aligned} \tag{1.41}$$

having introduced a parameter that counts how many states are occupied up to the one we want to change

$$\Sigma_i = \sum_{j=1}^{i-1} n_j. \tag{1.42}$$

1.9 Interactions

The natural generalization of second quantization to two body operators is

$$\hat{V} = \frac{1}{2} \int d^3x \int d^3x' \sum_{\sigma\sigma'} V(x - x') \hat{\psi}_{\sigma'}^\dagger(x') \hat{\psi}_\sigma^\dagger(x) \hat{\psi}_\sigma(x) \hat{\psi}_{\sigma'}(x') \tag{1.43}$$

The Fourier harmonics are

$$\hat{\psi}_\sigma(x) = \int \frac{d^3k}{(2\pi)^3} \, e^{ikx} \, \hat{c}_{k,\sigma} \,, \qquad \text{with } \{\hat{c}_{k,\sigma}, \; \hat{c}_{k',\sigma'}^\dagger\} = (2\pi)^3 \delta(k - k') \delta_{\sigma,\sigma'} \tag{1.44}$$

$$V(x - x') = \int \frac{d^3q}{(2\pi)^3} \, e^{iq(x - x')} \, V(q) \tag{1.45}$$

so in momentum space we can write the interaction as

$$\hat{V} = \frac{1}{2} \sum_{kk'q} \sum_{\sigma\sigma'} \hat{c}_{k+q,\sigma}^\dagger \hat{c}_{k'-q,\sigma'}^\dagger \hat{c}_{k',\sigma'} \hat{c}_{k,\sigma} \tag{1.46}$$

which is quite intuitive to understand: two particles are destroyed and two new particles are created with a momentum shift of q, that's the second quantization description of 2-particles collision!

1.10 Free electron gas

Consider an Hamiltonian where every mode has an energy $\epsilon_k = \frac{\hbar^2 k^2}{2m}$, such that

$$\hat{H}^0 = \sum_{k,\sigma} \epsilon_k \, \hat{c}_{k,\sigma}^\dagger \, \hat{c}_{k,\sigma} \tag{1.47}$$

From Solid State theory we know that at low temperatures ($T \lesssim 10^4 K$) the states occupied by an electron look like a sphere in momentum space (so called *Fermi sphere*), with radius k_F. We can construct a state called Ground State

$$|G\rangle = \prod_{|k| < k_F, \, \sigma} \hat{c}_{k,\sigma}^\dagger |0\rangle \tag{1.48}$$

We can relate the *Fermi momentum* k_F to the density of electrons taking the expectation value of $\hat{N}$ on the Ground State

$$N = \langle G|\sum_{k,\sigma} \hat{n}_{k,\sigma}|G\rangle = \sum_{\sigma} V \int \frac{d^3k}{(2\pi)^3} \langle G|\hat{n}_k|G\rangle \simeq$$
$$\simeq 2V \int \frac{d^3k}{(2\pi)^3} \theta(|k| - k_F) = 2V \frac{1}{(2\pi)^3} \frac{4\pi}{3} k_F^3$$

$$k_F^3 = 3\pi^2 \frac{N}{V} \tag{1.49}$$

In the same way we can get the average energy

$$E = \langle G|\hat{H}^0|G\rangle = \frac{2V}{(2\pi)^3} \int d^3k \frac{\hbar^2 k^2}{2m} \theta(|k| - k_F)$$
$$= \frac{V\hbar^2}{8\pi^3 m} 4\pi \int_0^{k_F} dk(k^4) = \frac{V\hbar^2}{2\pi^2 m} \frac{k_F^5}{5} = \frac{Vk_F^3}{5\pi^2} \epsilon_F = \frac{3}{5} N\epsilon_F$$

Appendix A - Spin $\frac{1}{2}$ Heisenberg chain

Single spin We can exploit the fact that the raising/lowering spin $\frac{1}{2}$ operators built out of Pauli matrices have the same algebra of fermionic creation/annihilation operators

$$\sigma_{\pm} = \frac{1}{\sqrt{2}}(\sigma_x \pm i\sigma_y)$$

$$\begin{aligned}\{\sigma_+, \sigma_-\} &= \frac{1}{2}\left[(\sigma_x + i\sigma_y)(\sigma_x - i\sigma_y) + (\sigma_x + i\sigma_y)(\sigma_x + i\sigma_y)\right] \\ &= \frac{1}{2}\left(\sigma_x^2 - i[\sigma_x, \sigma_y] + \sigma_y^2 + \sigma_x^2 + i[\sigma_x, \sigma_y] + \sigma_y^2\right) = 1.\end{aligned}$$

So now we call the spin raising/lowering operators $\hat{f}^\dagger, \hat{f}$ and we say that their action is

$$\hat{f}|\downarrow\rangle = \hat{f}|0\rangle = 0, \qquad \hat{f}^\dagger|\downarrow\rangle = |1\rangle = |\uparrow\rangle, \qquad \hat{f}^\dagger|\uparrow\rangle = 0 \tag{1.50}$$

In the representation where $|\uparrow\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, $|\downarrow\rangle = \begin{pmatrix}0\\1\end{pmatrix}$, the raising/lowering operators are 2-by-2 matrices

$$\hat{f}^\dagger = \begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}, \qquad \hat{f} = \begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix} \tag{1.51}$$

$$S^z = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = \begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix} - \frac{1}{2} = \hat{f}^\dagger\hat{f} - \frac{1}{2} \tag{1.52}$$

$$S^x = \frac{1}{2}(\hat{f}^\dagger + \hat{f}), \qquad S^y = \frac{1}{2i}(\hat{f}^\dagger - \hat{f}) \tag{1.53}$$

And we know the Cartesian components of the spin have the same commutation relations as angular momentum.

Many spins For many spins we need a more refined model, because if it were just for spins the ones on different sites of the chain would commute, while fermions would anti-commute. We perform a so called *Jordan-Wigner transformation*: for each site j we then define a new phase operator

$$\hat{\phi}_j = \pi\sum_{l<j}\hat{n}_l = \pi\sum_{l<j}\hat{f}_l^\dagger\hat{f}_l \tag{1.54}$$

such that the new spin ladder operators are a fermion times a *string* operator

$$S_j^+ = \hat{f}_j^\dagger e^{i\hat{\phi}_j}, \qquad S_j^- = \hat{f}_j e^{-i\hat{\phi}_j} \tag{1.55}$$

and the z-component is still

$$S_j^z = \hat{f}_j^\dagger\hat{f}_j - \frac{1}{2}. \tag{1.56}$$

It's important to note that the string operator is hermitian

$$e^{i\hat{\phi}_j} = e^{-i\hat{\phi}_j} \tag{1.57}$$

since the outcome of applying it to a state is either to leave it unvaried or to change the sign.

Let's study the algebra of these new operators. First we look at how the complex phase given by the occupation operator commute with fermions annihilation operators

$$\begin{aligned} e^{i\pi\hat{n}_j}\,\hat{f}_j|n_1,...,n_j,...\rangle &= e^{i\pi\hat{n}_j}\left[(-1)^{\sum_{l<j}n_l}n_j|n_1,...,n_j-1,...\rangle\right] \\ &= e^{i\pi(n_j-1)}\left[(-1)^{\sum_{l<j}n_l}n_j|n_1,...,n_j-1,...\rangle\right] \end{aligned} \tag{1.58}$$

$$\begin{aligned} \hat{f}_j\,e^{i\pi\hat{n}_j}|n_1,...,n_j,...\rangle &= \hat{f}_j\,\left[e^{i\pi n_j}|n_1,...,n_j,...\rangle\right] \\ &= e^{i\pi n_j}\left[(-1)^{\sum_{l<j}n_l}n_j|n_1,...,n_j-1,...\rangle\right] \end{aligned} \tag{1.59}$$

so they are the same except for a $e^{-i\pi}=-1$, which means they anti-commute

$$\rightarrow \{e^{i\pi\hat{n}_j}\,,\hat{f}_j\}=0 \tag{1.60}$$

Notice that $e^{i\pi\hat{n}_j}=e^{-i\pi\hat{n}_j}$, so if we take the hermitian conjugate of the last expression we get

$$\{e^{i\pi\hat{n}_j}\,,\hat{f}_j^\dagger\}=0 \tag{1.61}$$

Where instead for $l\neq j$ we would've gotten

$$\begin{aligned} e^{i\pi\hat{n}_l}\,\hat{f}_j|n_1,...,n_j,...\rangle &= e^{i\pi\hat{n}_l}\left[(-1)^{\sum_{l<j}n_l}n_j|n_1,...,n_j-1,...\rangle\right] \\ &= e^{i\pi n_l}\left[(-1)^{\sum_{l<j}n_l}n_j|n_1,...,n_j-1,...\rangle\right] \end{aligned} \tag{1.62}$$

$$\begin{aligned} \hat{f}_j\,e^{i\pi\hat{n}_l}|n_1,...,n_j,...\rangle &= \hat{f}_j\,\left[e^{i\pi n_j}|n_1,...,n_j,...\rangle\right] \\ &= e^{i\pi n_l}\left[(-1)^{\sum_{l<j}n_l}n_j|n_1,...,n_j-1,...\rangle\right] \end{aligned} \tag{1.63}$$

that are exactly the same, which means they commute

$$[e^{i\pi\hat{n}_l}\,,\hat{f}_j^\dagger]=0\,,\qquad [e^{i\pi\hat{n}_l}\,,\hat{f}_j^\dagger]=0\qquad \forall l\neq j \tag{1.64}$$

Finally, for the string operators we get, if $l\leq j$

$$\begin{aligned} e^{i\hat{\phi}_l}\,\hat{f}_j|n_1,...,n_j,...\rangle &= e^{i\pi\hat{n}_1}...e^{i\pi\hat{n}_{l-1}}\left[(-1)^{\sum_{k<j}n_k}n_j|n_1,...,n_j-1,...\rangle\right] \\ &= e^{i\pi(n_1+...+n_{l-1})}\left[(-1)^{\sum_{k<j}n_k}n_j|n_1,...,n_j-1,...\rangle\right] \\ &= e^{i\pi(n_1+...+n_{l-1})}e^{i\pi(n_1+...+n_l+...+n_{j-1})}n_j|n_1,...,n_j-1,...\rangle \\ &= e^{i\pi(n_l+...+n_{j-1})}n_j|n_1,...,n_j-1,...\rangle \end{aligned} \tag{1.65}$$

$$\begin{aligned} \hat{f}_j\,e^{i\hat{\phi}_l}|n_1,...,n_j,...\rangle &= \hat{f}_j\left[e^{i\pi(n_1+...+n_{l-1})}|n_1,...,n_j,...\rangle\right] \\ &= e^{i\pi(n_1+...+n_{l-1})}\left[(-1)^{\sum_{k<j}n_k}n_j|n_1,...,n_j-1,...\rangle\right] \\ &= e^{i\pi(n_1+...+n_{l-1})}e^{i\pi(n_1+...+n_{j-1})}n_j|n_1,...,n_j-1,...\rangle \\ &= e^{i\pi(n_l+...+n_{j-1})}n_j|n_1,...,n_j-1,...\rangle \end{aligned} \tag{1.66}$$

while if $l > j$

$$
\begin{aligned}
e^{i\hat{\phi}_l}\,\hat{f}_j|n_1,...,n_j,...\rangle &= e^{i\pi\hat{n}_1}...e^{i\pi\hat{n}_j}...e^{i\pi\hat{n}_{l-1}}\left[(-1)^{\sum_{k<j}n_k}n_j|n_1,...,n_j-1,...\rangle\right] \\
&= e^{i\pi(n_1+...+n_{l-1}-1)}\left[(-1)^{\sum_{k<j}n_k}n_j|n_1,...,n_j-1,...\rangle\right] \\
&= e^{i\pi(n_j+...+n_{l-1}-1)}n_j|n_1,...,n_j-1,...\rangle \\
&= -e^{i\pi(n_j+...+n_{l-1})}n_j|n_1,...,n_j-1,...\rangle
\end{aligned}
\tag{1.67}
$$

$$
\hat{f}_j\,e^{i\hat{\phi}_l}|n_1,...,n_j,...\rangle = e^{i\pi(n_j+...+n_{l-1})}n_j|n_1,...,n_j-1,...\rangle. \tag{1.68}
$$

and we would get the same results for $\hat{f}_j^\dagger$. So in general we get

$$
[e^{i\hat{\phi}_l}\,,\hat{f}_j] = [e^{i\hat{\phi}_l}\,,\hat{f}_j^\dagger] = 0\,, \qquad \text{if } l \leq j \tag{1.69}
$$

$$
\{e^{i\hat{\phi}_l}\,,\hat{f}_j\} = \{e^{i\hat{\phi}_l}\,,\hat{f}_j^\dagger\} = 0\,, \qquad \text{if } l > j \tag{1.70}
$$

Now we can confirm that our choice of writing the spin ladder operator as the product of a string times a fermionic creation/annihilation operator was right. We need for the spin ladder operators of different sites to commute

$$
[S_j^\pm\,,S_k^\pm] = [\hat{f}_j^{(\dagger)}e^{i\hat{\phi}_j}\,,\hat{f}_k^{(\dagger)}e^{i\hat{\phi}_k}] = [e^{i\hat{\phi}_j}\hat{f}_j^{(\dagger)}\,,\hat{f}_k^{(\dagger)}e^{i\hat{\phi}_k}] \tag{1.71}
$$

if $j < k$

$$
\begin{aligned}
[S_j^\pm\,,S_k^\pm] &= e^{i\hat{\phi}_j}[\hat{f}_j^{(\dagger)}\,,\hat{f}_k^{(\dagger)}e^{i\hat{\phi}_k}] + \overbrace{[e^{i\hat{\phi}_j}\,,\hat{f}_k^{(\dagger)}e^{i\hat{\phi}_k}]\hat{f}_j^{(\dagger)}}^{[\hat{\phi}_j\,,\hat{\phi}_k]=0\,,[e^{i\hat{\phi}_j}\,,\hat{f}_k^{(\dagger)}]=0} \\
&= e^{i\hat{\phi}_j}\underbrace{\{\hat{f}_j^{(\dagger)}\,,\hat{f}_k^{(\dagger)}\}}_{=0,\text{ fermions}}e^{i\hat{\phi}_k} - e^{i\hat{\phi}_j}\hat{f}_k^{(\dagger)}\underbrace{\{\hat{f}_j^{(\dagger)}\,,e^{i\hat{\phi}_k}\}}_{=0} = 0
\end{aligned}
\tag{1.72}
$$

while if $j > k$

$$
\begin{aligned}
[S_j^\pm\,,S_k^\pm] &= e^{i\hat{\phi}_j}\overbrace{\{\hat{f}_j^{(\dagger)}\,,\hat{f}_k^{(\dagger)}\}}^{=0,\text{ fermions}}e^{i\hat{\phi}_k} - e^{i\hat{\phi}_j}\hat{f}_k^{(\dagger)}\overbrace{\{\hat{f}_j^{(\dagger)}\,,e^{i\hat{\phi}_k}\}}^{=2e^{i\hat{\phi}_k}\hat{f}_j^{(\dagger)}} \\
&\quad + \underbrace{\{e^{i\hat{\phi}_j}\,,\hat{f}_k^{(\dagger)}\}}_{=0}e^{i\hat{\phi}_k}\hat{f}_j^{(\dagger)} - \hat{f}_k^{(\dagger)}\underbrace{\{e^{i\hat{\phi}_j}\,,e^{i\hat{\phi}_k}\}}_{=2e^{i\hat{\phi}_j}e^{i\hat{\phi}_k}}\hat{f}_j^{(\dagger)} \\
&= 2\hat{f}_k^{(\dagger)}e^{i\hat{\phi}_j}e^{i\hat{\phi}_k}\hat{f}_j^{(\dagger)} - 2\hat{f}_k^{(\dagger)}e^{i\hat{\phi}_j}e^{i\hat{\phi}_k}\hat{f}_j^{(\dagger)} = 0.
\end{aligned}
\tag{1.73}
$$

Now we study the spin-spin ferromagnetic interaction

$$
H = -\frac{J}{2}\sum_j\left(S_{j+1}^+S_j^- + S_j^+S_{j+1}^-\right) - J_z\sum_j S_{j+1}^zS_j^z \tag{1.74}
$$

substituting the fermionic and string operators (*Fermionization*)

$$
\begin{aligned}
H &= -\frac{J}{2}\sum_j\left(\hat{f}_{j+1}^\dagger e^{i\hat{\phi}_{j+1}}e^{i\hat{\phi}_j}\hat{f}_j + \hat{f}_j^\dagger e^{i\hat{\phi}_j}e^{i\hat{\phi}_{j+1}}\hat{f}_{j+1}\right) - J_z\sum_j\left(\hat{n}_{j+1}-\frac{1}{2}\right)\left(\hat{n}_j-\frac{1}{2}\right) \\
&= -\frac{J}{2}\sum_j\left(\hat{f}_{j+1}^\dagger e^{i\pi\hat{n}_j}\hat{f}_j + \hat{f}_j^\dagger e^{i\pi\hat{n}_j}\hat{f}_{j+1}\right) - J_z\sum_j\left(\hat{n}_{j+1}\hat{n}_j - \frac{1}{2}\hat{n}_j - \frac{1}{2}\hat{n}_{j+1} + \frac{1}{4}\right)
\end{aligned}
\tag{1.75}
$$

In the first term $\hat{f}^{\dagger}_{j+1}e^{i\pi\hat{n}_j}\hat{f}_j$ we are annihilating a particle in site j so the occupation number is $n_j = 0$ and $e^{i\pi\hat{n}_j} = 1$. For the opposite reason, in the second term $\hat{f}^{\dagger}_j e^{i\pi\hat{n}_j}\hat{f}_{j+1}$ we are creating a particle in site j so the occupation number has to be $n_j = 0$ in order to not give zero when $f^{\dagger}_j$ is applied to it, this means $e^{i\pi\hat{n}_j} = 1$. Ignoring the constant term we finally get

$$H = -\frac{J}{2}\sum_j \left(\hat{f}^{\dagger}_{j+1}\hat{f}_j + \hat{f}^{\dagger}_j\hat{f}_{j+1}\right) + J_z\sum_j \hat{n}_j - J_z\sum_j \hat{n}_j\hat{n}_{j+1} \tag{1.76}$$

so the xy-component of the Hamiltonian becomes an "hopping" term, there's a probability amplitude that a particle will be annihilated on one site and created in a neighboring one.

2 Second Quantization Perturbation theory

2.1 Interaction picture

If the Hamiltonian is made up of the free one plus a perturbation $H = H_0 + V$, we define the states and operators in the Interaction (or sometimes called Dirac) picture to be

$$\begin{aligned} |\psi_I(t)\rangle &= e^{iH_0 t}|\psi(t)\rangle \\ O_I(t) &= e^{iH_0 t} O e^{-iH_0 t} \end{aligned} \tag{2.1}$$

If we now look at the time evolution of the state

$$\begin{aligned} |\psi(t)\rangle &= e^{-iHt}|\psi(t')\rangle = e^{-iHt}e^{iHt'}|\psi(t')\rangle \\ e^{iH_0 t}|\psi(t)\rangle &= e^{iH_0 t}e^{-iHt}e^{iHt'}e^{-iH_0 t'}|\psi_I(t')\rangle \\ \rightarrow |\psi_I(t)\rangle &= U(t)U^\dagger(t')|\psi_I(t')\rangle \\ &= S(t,t')|\psi_I(t')\rangle \end{aligned} \tag{2.2}$$

where we have defined S(t,t') to be the *Scattering matrix.* The time evolution of $U(t)$ is

$$\begin{aligned} i\frac{\partial U(t)}{\partial t} &= i\frac{\partial}{\partial t}\left(e^{iH_0 t}e^{-iHt}\right) \\ &= -e^{iH_0 t}H_0 e^{-iHt} + e^{iH_0 t}He^{-iHt} \\ &= e^{iH_0 t}Ve^{-iHt} \\ &= \underbrace{e^{iH_0 t}Ve^{-iH_0 t}}_{=V_I(t)}\underbrace{e^{iH_0 t}e^{-iHt}}_{=U(t)} = V_I(t)U(t) \end{aligned} \tag{2.3}$$

so it's also true for the states

$$i\frac{\partial}{\partial t}|\psi_I(t)\rangle = V_I(t)|\psi_I(t)\rangle \tag{2.4}$$

and for the Scattering matrix

$$i\frac{\partial}{\partial t}S(t,t') = V_I(t)S(t,t') \tag{2.5}$$

but from now on we'll always assume operators to be in the Interaction picture.

How do we solve 2.5? If we just try to integrate we get the recursive equation

$$\begin{aligned} S(t,t') &= \mathbb{1} - i\int_{t'}^{t} dt_1 V_I(t_1)S(t_1,t') \\ &= \mathbb{1} - i\int_{t'}^{t} dt_1 V_I(t_1)\left(\mathbb{1} - i\int_{t'}^{t_1} dt_2 V_I(t_2)S(t_2,t')\right) \\ &= \mathbb{1} - i\int_{t'}^{t} dt_1 V_I(t_1) - \int_{t'}^{t} dt_1\int_{t'}^{t_1} dt_2 V_I(t_1)V_I(t_2) + O(V^3) \end{aligned} \tag{2.6}$$

Let's look at the second order of the expansion in more detail

$$\int_{t'}^{t} dt_1 \int_{t'}^{t_1} dt_2 V_I(t_1)V_I(t_2) = \frac{1}{2}\left[\int_{t'}^{t} dt_1 \int_{t'}^{t_1} dt_2 V_I(t_1)V_I(t_2) + \int_{t'}^{t} dt_1 \int_{t'}^{t_1} dt_2 V_I(t_1)V_I(t_2)\right]$$
$$= \frac{1}{2}\left[\int_{t'}^{t} dt_1 \int_{t'}^{t} dt_2 V_I(t_1)V_I(t_2)\Theta(t_1-t_2) + \int_{t'}^{t} dt_2 \int_{t'}^{t} dt_1 V_I(t_2)V_I(t_1)\Theta(t_2-t_1)\right]$$
$$= \frac{1}{2}\int_{t'}^{t} dt_1 \int_{t'}^{t} dt_2 \left[V_I(t_1)V_I(t_2)\Theta(t_1-t_2) + V_I(t_2)V_I(t_1)\Theta(t_2-t_1)\right] \tag{2.7}$$

which is the definition of *time ordering* for bosons, so

$$\int_{t'}^{t} dt_1 \int_{t'}^{t_1} dt_2 V_I(t_1)V_I(t_2) = \frac{1}{2}\int_{t'}^{t} dt_1 \int_{t'}^{t} dt_2 T[V_I(t_1)V_I(t_2)] \tag{2.8}$$

Time ordering Given an ordered set of operators at different times $\{O_1(t_1), ..., O_N(t_N)\}$, we define the *time ordering operator* to act like this on the product of the operators:

$$T[O_1(t_1)\,...O_N(t_N)] = \begin{cases} O_{P_1}(t_{P_1})\,...O_{P_N}(t_{P_N}) \\ \mathrm{sgn}(P)O_{P_1}(t_{P_1})\,...O_{P_N}(t_{P_N}) \end{cases} \tag{2.9}$$

where P is the permutation that orders the operators with respect to time: $t_{P_1} > \,...\, > t_{P_N}$. It can be shown (via induction) that every order of the expansion can be written in terms of time ordered powers of V_I, such that

$$S(t,t') = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{t'}^{t} dt_1 ... \int_{t'}^{t} dt_n T[V_I(t_1)\,...V_I(t_n)] \equiv T\, e^{-i\int_{t'}^{t} d\tau V_I(\tau)} \tag{2.10}$$

if you want to sound like a person who has nice geometrical intuitions you can say that the factorial on the denominator comes out because we're "just integrating on triangles".

2.2 Driven harmonic oscillator

Consider a parturbation V(t) to the hamiltonian of the harmonic oscillator

$$H_0 = \omega\left(b^\dagger b + \frac{1}{2}\right), \qquad V(t) = \bar{z}(t)b + b^\dagger z(t). \tag{2.11}$$

We are interested in calculating the probability amplitude that the system is starting in the ground state in the remote past and it's still there in the distant future

$$\langle 0|S(\infty, -\infty)|0\rangle = \langle 0|T\, e^{-i\int_{-\infty}^{\infty} dt[\bar{z}(t)b + b^\dagger z(t)]}|0\rangle \equiv S[\bar{z}, z] \tag{2.12}$$

where we look at S as a funtional of $\bar{z}(t), z(t)$. If we were considering just a finite interval $[-\tau, \tau]$ we could divide it into N pieces of equal length $[\tau_0, \tau_1]$, $...[\tau_{N-1}, \tau_N]$, with $\tau_j = -\tau + j\frac{2\tau}{N} = -\tau + j\Delta\tau$

$$S(\tau, -\tau) = S(\tau_N, \tau_{N-1})\, ...S(\tau_1, \tau_0) \tag{2.13}$$

and if $\Delta\tau \ll 2\tau$ we can approximate

$$S(\tau_n, \tau_{n-1}) \approx e^{-iV(\tau_n)\Delta\tau + O(\Delta\tau^2)} \tag{2.14}$$

such that we introduce a new quantity S_N that will converge to $S(\tau - \tau)$ for small time steps

$$S_N \equiv e^{-iV(\tau_N)\Delta\tau} e^{-iV(\tau_{N-1})\Delta\tau} ...e^{-iV(\tau_1)\Delta\tau} \xrightarrow[\Delta\tau \to 0]{} S(\tau, -\tau). \tag{2.15}$$

We now write the exponents as a difference of two new operators

$$A_r = -i\bar{z}(\tau_r)b(\tau_r)\Delta\tau\,, \qquad A_r^\dagger = iz(\tau_r)b^\dagger(\tau_r)\Delta\tau \tag{2.16}$$

$$-\, iV(\tau_r)\Delta\tau \equiv A_r - A_r^\dagger \tag{2.17}$$

$$S_N = e^{(A_N - A_N^\dagger)}\, ...e^{(A_1 - A_1^\dagger)} \tag{2.18}$$

where we remember the time evolution of the creation/annihilation operators is

$$b(\tau_r) = be^{-i\omega\tau_r}\,, \qquad b^\dagger(\tau_r) = b^\dagger e^{i\omega\tau_r}. \tag{2.19}$$

The commutator $[A_r, A_r^\dagger] = \hat{z}(\tau_r)z(\tau_r)[b(\tau_r), b^\dagger(\tau_r)](\Delta\tau)^2 = \hat{z}(\tau_r)z(\tau_r)(\Delta\tau)^2$ is a c-number, so according to the BCH formula

$$e^{A_r - A_r^\dagger - [A_r, A_r^\dagger]/2} = e^{A_r} e^{-A_r^\dagger} \tag{2.20}$$

$$e^{-A_r^\dagger + A_r - [A_r^\dagger, A_r]/2} = e^{-A_r^\dagger} e^{A_r} \tag{2.21}$$

$$e^{A_r - A_r^\dagger} = e^{A_r} e^{-A_r^\dagger} e^{[A_r, A_r^\dagger]/2} = e^{-A_r^\dagger} e^{A_r} e^{-[A_r, A_r^\dagger]/2} \tag{2.22}$$

where we can stop at second order because higher orders are zero, given that they would contain commutators between an operator and (the identity times) a number. Putting 2.22 in S_N we get

$$S_N = e^{-A_N^\dagger} e^{A_N}\, ...e^{-A_1^\dagger} e^{A_1} e^{-\sum_r [A_r, A_r^\dagger]/2}. \tag{2.23}$$

Let's now look at the commutator for different indices

$$
\begin{aligned}
[A_r, A_s^\dagger] &= (\Delta\tau)^2 \bar{z}(\tau_r) z(\tau_s) [b e^{-i\omega\tau_r}, b^\dagger e^{i\omega\tau_s}] \\
&= (\Delta\tau)^2 \bar{z}(\tau_r) z(\tau_s)\, e^{-i\omega(\tau_r - \tau_s)},
\end{aligned} \tag{2.24}
$$

we would like to move all the terms in 2.23 with A_r to the right of the terms with $-A_r^\dagger$, so using again 2.22 (but with different indices)

$$
e^{A_r} e^{-A_s^\dagger} = e^{-A_s^\dagger} e^{A_r} e^{-[A_r, A_s^\dagger]} \tag{2.25}
$$

and substituting this into S_N a lot of times, we can get

$$
\begin{aligned}
S_N &= e^{-A_N^\dagger} e^{A_N} \ldots e^{-A_3^\dagger} e^{A_3} e^{-A_2^\dagger} \underbrace{e^{A_2} e^{-A_1^\dagger}} e^{A_1} e^{-\sum_r [A_r, A_r^\dagger]/2} \\
&= e^{-A_N^\dagger} e^{A_N} \ldots e^{-A_3^\dagger} \underbrace{e^{A_3} e^{-A_2^\dagger}} e^{-A_1^\dagger} e^{A_2} e^{A_1} e^{-\sum_r [A_r, A_r^\dagger]/2} e^{-[A_2, A_1^\dagger]} \\
&= e^{-A_N^\dagger} e^{A_N} \ldots e^{-A_3^\dagger} e^{-A_2^\dagger} \underbrace{e^{A_3} e^{-A_1^\dagger}} e^{A_2} e^{A_1} e^{-\sum_r [A_r, A_r^\dagger]/2} e^{-[A_2, A_1^\dagger] - [A_3, A_2^\dagger]} \\
&= e^{-A_N^\dagger} e^{A_N} \ldots e^{-A_3^\dagger} e^{-A_2^\dagger} e^{-A_1^\dagger} e^{A_3} e^{A_2} e^{A_1} e^{-\sum_r [A_r, A_r^\dagger]/2} e^{-[A_2, A_1^\dagger] - [A_3, A_2^\dagger] - [A_3, A_1^\dagger]} \\
&\vdots \\
&= e^{-\sum_r A_r^\dagger} e^{\sum_r A_r} e^{-\sum_r [A_r, A_r^\dagger]/2} e^{-\sum_{r>s} [A_r, A_s^\dagger]} \\
&= e^{-\sum_r A_r^\dagger} e^{\sum_r A_r} e^{-\sum_{r \geq s} (1 - \delta_{rs}/2) [A_r, A_s^\dagger]}
\end{aligned} \tag{2.26}
$$

where we've also used the fact that $[A_r^\dagger, A_s^\dagger] = [A_r, A_s] = 0$.
Let's look for a moment at what is the action of the operators A_r, $A_r^\dagger$ on the vacuum. Using the properties of the creation/annihilation operators $b|0\rangle = 0$ and $\langle 0| b^\dagger = 0$, from 2.16 we see that the same holds for A_r, $A_r^\dagger$

$$
A_r |0\rangle = -i\bar{z}(\tau_r) e^{-i\omega\tau_r} b |0\rangle = 0\,, \qquad \langle 0| A_r^\dagger = \langle 0| b^\dagger i z(\tau_r) e^{i\omega\tau_r} = 0 \tag{2.27}
$$

so when we exponentiate them we get

$$
\begin{aligned}
e^{A_r} |0\rangle &= \left(\mathbb{1} + A_r + \frac{1}{2} A_r^2 + \ldots \right) |0\rangle = |0\rangle\,, \\
\langle 0| e^{-A_r^\dagger} &= \langle 0| \left(\mathbb{1} - A_r + \frac{1}{2} (A_r^\dagger)^2 + \ldots \right) = \langle 0|.
\end{aligned} \tag{2.28}
$$

We now have all the ingredients to consider the expectation value on the vacuum[1]

$$
\begin{aligned}
\langle 0| S_N |0\rangle &= \langle 0| e^{-\sum_r A_r^\dagger} e^{\sum_r A_r} |0\rangle e^{-\sum_{r \geq s} (1 - \delta_{rs}/2) [A_r, A_s^\dagger]} \\
&= \langle 0| \prod_r e^{-A_r^\dagger} \prod_r e^{A_r} |0\rangle e^{-\sum_{r \geq s} (1 - \delta_{rs}/2) [A_r, A_s^\dagger]} \\
&= \langle 0|0\rangle e^{-\sum_{r \geq s} (1 - \delta_{rs}/2) [A_r, A_s^\dagger]} \\
&= e^{-\sum_{r \geq s} (1 - \delta_{rs}/2) (\Delta\tau)^2 \bar{z}(\tau_r) z(\tau_s)\, e^{-i\omega(\tau_r - \tau_s)}}
\end{aligned} \tag{2.29}
$$

[1]We can switch from $e^{\sum_r A_r}$ to $\prod_r e^{A_r}$ because in the BCH formula we don't get any extra term given by commutators, since $[A_r, A_s] = 0$. The same holds for $A_r^\dagger$.

where in the end we have substituted the value of the commutator 2.24.
Taking the continuum limit for $N \to \infty$ (that is $\Delta\tau \to 0$) we can turn the double sum constrained on times $\tau_r \geq \tau_s$ into a double integral with a step function that constrains the integration on times $t > t'$. Also we have that $\delta_{rs} \to \Delta\tau\delta(t-t')$[2], so when $\Delta\tau$ goes to zero, we can ignore this term

$$\langle 0|S(\tau,-\tau)|0\rangle = \exp\left\{-\int_{-\tau}^{\tau} dt \int_{-\tau}^{\tau} dt' \bar{z}(t)\Theta(t-t')e^{-i\omega(t-t')}z(t')\Big(1-\underbrace{\Delta\tau\delta(t-t')}_{\to 0}\Big)\right\} \tag{2.30}$$

and at last we can take the limit $\tau \to \infty$

$$\boxed{S[\bar{z},z] \equiv \langle 0|S(\infty,-\infty)|0\rangle = e^{-i\int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' \bar{z}(t)G(t-t')z(t')}} \tag{2.31}$$

where we define the so called *one particle Green's function* as

$$G(t-t') = -i\Theta(t-t')\, e^{-i\omega(t-t')}. \tag{2.32}$$

2.3 Wick's theorem

Taking functional derivatives of $S[\bar{z},z]$ with respect to $\bar{z}$ and z gives us

$$\begin{aligned} \frac{\delta}{\delta\bar{z}(t)}S &= \frac{\delta}{\delta\bar{z}(t)}e^{-i\int dt \int dt' \bar{z}(t)G(t-t')z(t')} \\ &= S\times\left\{-i\int dt' G(t-t')z(t')\right\} \\ \frac{\delta^2}{\delta z(t')\delta\bar{z}(t)}S\bigg|_{\bar{z},z=0} &= -iG(t-t') \end{aligned} \tag{2.33}$$

but also

$$\begin{aligned} \frac{\delta}{\delta\bar{z}(t)}S &= \frac{\delta}{\delta\bar{z}(t)}\langle 0|T\, e^{-i\int dt'[\bar{z}(t')b+b^\dagger z(t')]}|0\rangle \\ &= -i\langle 0|\hat{S}b(t)|0\rangle \\ \frac{\delta^2}{\delta z(t')\delta\bar{z}(t)}S\bigg|_{\bar{z},z=0} &= -\langle 0|Tb(t)b^\dagger(t')|0\rangle \end{aligned} \tag{2.34}$$

so we get an operatorial expression for the Green's function

$$G(t-t') = -i\langle 0|Tb(t)b^\dagger(t')|0\rangle. \tag{2.35}$$

In general we could take a 2n-order derivative

$$\begin{aligned} \frac{\delta^{2n}}{\delta z(1')\delta z(2')...\delta\bar{z}(1)\delta\bar{z}(2)}S\bigg|_{\bar{z},z=0} &= -\langle 0|Tb(1)b(2)...b^\dagger(2')b^\dagger(1')|0\rangle \\ &= (-i)^n G(1,2,...n;1',2',...,n') \end{aligned} \tag{2.36}$$

[2]To convince yourself of this, look for example at Coleman's equation 2.111, where $\Delta q = \frac{2\pi}{L}$, so even there he got $\delta_{qq'} \to \Delta q\delta(q-q')$. In our case though, we're treating times instead of momenta so we have to multiply our Dirac's delta by the time step $\Delta\tau$.

where the last one is the n-particle Green's function

$$G(1,2,...2n;1',2',...,2n') = (-i)^n \langle 0|Tb(1)b(2)...b^\dagger(2')b^\dagger(1')|0\rangle. \tag{2.37}$$

Let's say we differentiate 2 times with respect to $\bar{z}$ and then 2 times with respect to z

$$\frac{\delta^2}{\delta\bar{z}(2)\delta\bar{z}(1)}S = S[\bar{z},z]\times(-i)^2[(G\circ z)(1)]\times[(G\circ z)(2)] \tag{2.38}$$

$$\begin{aligned}\frac{\delta^3}{\delta z(1')\delta\bar{z}(2)\delta\bar{z}(1)}S =& S[\bar{z},z]\times(-i)^2\Big\{-i[(\bar{z}\circ G)(1')]\times[(G\circ z)(1)]\times[(G\circ z)(2)]+\\ &+G(1-1')\times[(G\circ z)(2)]+[(G\circ z)(2)]\times G(2-1')\Big\}\end{aligned} \tag{2.39}$$

$$\frac{\delta^4}{\delta z(1')\delta z(2')\delta\bar{z}(2)\delta\bar{z}(1)}S\bigg|_{\bar{z},z=0} = (-i)^2\Big\{G(1-1')G(2-2')+G(2-1')G(2-2')\Big\} \tag{2.40}$$

so the 2-particle Green's function is

$$G(1,2;1',2') = G(1-1')G(2-2')+G(2-1')G(1-2'). \tag{2.41}$$

In general, for the n-particle Green's function, we would get the sum over all the permutations

$$G(1,2,...,n;1',2',...,n') = \sum_P\prod_s G(s-P'_s) \tag{2.42}$$

with this result being known as *Wick's Theorem*[3].

2.4 Green's functions

Up to now we've considered Green's functions for a single harmonic oscillator, in the *many body* case we need more degrees of freedom. The one particle Green's function can be written as

$$G_{\lambda\lambda'}(t-t') = -i\langle\phi|T\psi_\lambda(t)\psi^\dagger_{\lambda'}(t')|\phi\rangle \tag{2.43}$$

with ϕ being the many-body ground state and $\psi(t)$ is the field in the Heisenberg representation and

$$T\psi_\lambda(t)\psi^\dagger_{\lambda'}(t') = \begin{cases}\psi_\lambda(t)\psi^\dagger_{\lambda'}(t') & t>t'\\ \\ \pm\psi^\dagger_{\lambda'}(t')\psi_\lambda(t) & t'>t\text{ , bosons/fermions.}\end{cases} \tag{2.44}$$

For example in a traslationally invariant systems can use spin and momentum as indices

$$\begin{aligned}G_{k\sigma,k'\sigma'}(t-t') &= \delta_{kk'}\delta_{\sigma\sigma'}G(k,t-t') = (2\pi)^3\delta^3(k-k')\delta_{\sigma\sigma'}G(k,t-t')\\ &= -i(2\pi)^3\delta^3(k-k')\delta_{\sigma\sigma'}\langle\phi|T\psi_{k\sigma}(t)\psi^\dagger_{k\sigma}(t')|\phi\rangle\end{aligned} \tag{2.45}$$

[3]Despite the anglopohonic sounding name, my man Gian Carlo Wick was an Italian physicist.

whereas in real space it would become

$$
\begin{aligned}
G_{\sigma\sigma'}(x-x',t-t') &= \delta_{\sigma\sigma'}G(x-x',t-t') \\
&= -i\delta_{\sigma\sigma'}\langle\phi|T\psi_\sigma(x,t)\psi^\dagger_\sigma(x',t')|\phi\rangle
\end{aligned}
\tag{2.46}
$$

of course the relation between the field operators in the two representations is

$$
\psi_\sigma(x,t) = \int_k \psi_{k\sigma}(t)e^{ikx} \tag{2.47}
$$

so we can connect the two representations of the Green's function

$$
\begin{aligned}
G(x-x',t) &= -i\int_k\int_{k'}\langle\phi|T\psi_{k\sigma}(t)\psi^\dagger_{k'\sigma}(0)|\phi\rangle e^{i(kx-k'x')} \\
&= \int_k\int_{k'}\delta_{kk'}G(k,t-t')e^{i(kx-k'x')} \\
&= \int_k G(k,t-t')e^{ik(x-x')}.
\end{aligned}
\tag{2.48}
$$

We could even Fourier transform the time dependency

$$
G(k,t) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}G(k,\omega)e^{-i\omega t} \tag{2.49}
$$

$$
G(k,\omega) = \int_{-\infty}^{\infty} dtG(k,t)e^{i\omega t} \tag{2.50}
$$

which we will call the *propagator*, so that we can relate the amplitute probabilty in real space-time to it by

$$
\begin{aligned}
G(x-x',t-t') &= \int\frac{d^3k\,d\omega}{(2\pi)^4}G(k,\omega)e^{i[k(x-x')-\omega(t-t')]} \\
&= -i\langle\phi|T\psi_\sigma(x,t)\psi^\dagger_\sigma(x',t')|\phi\rangle
\end{aligned}
\tag{2.51}
$$

2.5 Free fermions case

Taking a gas of free fermions in its ground state $|\phi\rangle$ at T_0, in the grand-canonical ensamble we have

$$
H_0 - \mu N = \sum_{k,\sigma}\epsilon_k c^\dagger_{k\sigma}ck\sigma\,, \qquad \epsilon_k = \frac{\hbar^2k^2}{2m} - \epsilon_F \tag{2.52}
$$

with the ground state being

$$
|\phi\rangle = \prod_{|k|<k_F,\sigma} c^\dagger_{k\sigma}|0\rangle. \tag{2.53}
$$

We want to write the Green's function, which we know takes the form

$$
G(k,t-t') = -i\langle\phi|Tc_{k\sigma}(t)c^\dagger_{k\sigma}(t')|\phi\rangle\,, \tag{2.54}
$$

where the effect of the time-ordering operator is

$$
Tc_{k\sigma}(t)c^\dagger_{k'\sigma'}(t') = c_{k\sigma}(t)c^\dagger_{k'\sigma'}(t')\Theta(t-t') - c^\dagger_{k'\sigma'}(t')c_{k\sigma}(t)\Theta(t'-t)\,. \tag{2.55}
$$

The time evolution of the operators is

$$c^\dagger_{k\sigma}(t) = c^\dagger_{k\sigma} e^{i\epsilon_k t}\,, \qquad c_{k\sigma}(t) = c_{k\sigma} e^{-i\epsilon_k t} \tag{2.56}$$

so the expectation value on the ground state, if $t > t'$

$$\begin{aligned}\langle\phi|c_{k\sigma}(t)c^\dagger_{k'\sigma'}(t')|\phi\rangle &= \delta_{\sigma\sigma'}\delta_{kk'}e^{-i\epsilon_k(t-t')}\langle\phi|c_{k\sigma}c^\dagger_{k\sigma}|\phi\rangle \\ &= \delta_{\sigma\sigma'}\delta_{kk'}e^{-i\epsilon_k(t-t')}\langle\phi|1 - c^\dagger_{k\sigma}c_{k\sigma}|\phi\rangle \\ &= \delta_{\sigma\sigma'}\delta_{kk'}e^{-i\epsilon_k(t-t')}(1 - n_k)\end{aligned} \tag{2.57}$$

while if $t < t'$

$$\langle\phi|c^\dagger_{k'\sigma'}(t')c_{k\sigma}(t)|\phi\rangle = \delta_{\sigma\sigma'}\delta_{kk'}e^{-i\epsilon_k(t-t')}n_k\,. \tag{2.58}$$

Putting everything inside 2.54 we get, for the case of $t' = 0$

$$\begin{aligned}G(k,t) &= -i\, e^{-i\epsilon_k t}\Big[(1-n_k)\Theta(t) - n_k\Theta(-t)\Big] \\ &= -i\, e^{-i\epsilon_k t}\Big[\Theta(k-k_F)\Theta(t) - \Theta(k_F-k)\Theta(-t)\Big]\end{aligned} \tag{2.59}$$

where the first term is the forward propagation of a particle, while the second term is the backwards propagation of an hole. We can put them both in a single expression such as

$$G(k,t) = \begin{cases} -i\, e^{-i\epsilon_k t}\Theta(k-k_F) \;\; t > 0\,, \\ \\ \;\; i\, e^{-i\epsilon_k t}\Theta(k_F-k) \;\;\; t < 0\,. \end{cases} \tag{2.60}$$

Now we can Fourier transform the time dependence to get the propagator

$$\begin{aligned}G(k,\omega) &= -i\int_{-\infty}^{\infty} dt e^{i(\omega-\epsilon_k)t}\Big[\Theta(k-k_F)\Theta(t)e^{-\delta t} - \Theta(k_F-k)\Theta(-t)e^{\delta t}\Big] \\ &= -i\Theta(k-k_F)\int_0^\infty dt e^{i(\omega-\epsilon_k+i\delta)t} + i\Theta(k_F-k)\int_{-\infty}^0 dt e^{i(\omega-\epsilon_k-i\delta)t} \\ &= -i\left\{\frac{-\Theta(k-k_F)}{i(\omega-\epsilon_k+i\delta)} - \frac{\Theta(k_F-k)}{i(\omega-\epsilon_k-i\delta)}\right\} \\ &= \frac{\Theta(k-k_F)}{\omega-\epsilon_k+i\delta} + \frac{\Theta(k_F-k)}{\omega-\epsilon_k-i\delta} = \frac{1}{\omega-\epsilon_k\pm i\delta} \qquad \begin{cases} + \text{ if } k > k_F\,, \\ - \text{ if } k < k_F\,. \end{cases}\end{aligned} \tag{2.61}$$

where we added a regularization term to avoid infinities, but ultimately we would like to have $\delta \to 0$. Another short-hand notation could be

$$G(k,\omega) = \frac{1}{\omega-\epsilon_k+i\delta_k}\,, \qquad \delta_k = \mathrm{sgn}(k-k_F)\delta \tag{2.62}$$

Exercise - Calculating the average density of fermions with spin s

$$\langle\hat\rho(x)\rangle = \langle\phi|\sum_\sigma \psi^\dagger_\sigma(x)\psi_\sigma(x)|\phi\rangle \tag{2.63}$$

The trick is to write the operators as slightly delayed in time and then introduce the time-ordering operator, to make it become a Green's function. Since in the Green's function we would have $T\psi(t)\psi^\dagger(0)$, the time-ordering operator will commute them (and add a minus sign) if t is an earlier time then 0, so let's make t a very small negative number $-\delta$

$$\begin{aligned}\langle\hat\rho(x)\rangle &= \sum_\sigma \langle\phi|\psi^\dagger_\sigma(x,0)\psi_\sigma(x,0^-)|\phi\rangle \\ &= -\lim_{\delta\to 0}\sum_\sigma \langle\phi|T\psi_\sigma(x,-\delta)\psi^\dagger_\sigma(x,0)|\phi\rangle \\ &= -i(2s+1)\lim_{\delta\to 0}\underbrace{G(0;-\delta)}_{G(x-x;-\delta-0)} .\end{aligned} \tag{2.64}$$

Let's now calculate the Green's function as the Fourier transform of the propagator as in 2.51

$$\begin{aligned}G(0;-\delta) &= \int\frac{d^3k\,d\omega}{(2\pi)^4}G(k,\omega)e^{i\omega\delta} = \int\frac{d^3k\,d\omega}{(2\pi)^4}\frac{e^{i\omega\delta}}{\omega-\epsilon_k+i\delta_k} \\ &= \int\frac{d^3k}{(2\pi)^4}\Theta(k_F-k)2\pi i\ \mathrm{Res}\left[\frac{e^{i\omega\delta}}{\omega-\epsilon_k-i\delta_k}\ ;\ \ \omega=\epsilon_k+i\delta\right]\end{aligned} \tag{2.65}$$

where $\delta>0$ so we need to close the integration in the upper complex semi-plane, so we only take the $k>k_F$ part of the propagator and pick up the residues of the poles with positive imaginary part

$$\begin{aligned}G(0;-\delta) &= \int\frac{d^3k}{(2\pi)^4}\Theta(k_F-k)\,2\pi i\lim_{\omega\to\epsilon_k+i\delta}(\omega-\epsilon_k-i\delta)\frac{e^{i\omega\delta}}{\omega-\epsilon_k-i\delta} \\ &\xrightarrow[\delta\to 0]{}\ i\frac{4\pi}{8\pi^3}\int k^2dk\,\Theta(k_F-k) = \frac{i}{8\pi^3}\frac{4\pi}{3}k_F^3 = i\frac{k_F^3}{6\pi^2} .\end{aligned} \tag{2.66}$$

Putting this back into 2.64 we finally get

$$n \equiv \langle\hat\rho(x)\rangle = (2s+1)\frac{k_F^3}{6\pi^2} \tag{2.67}$$

so for electrons (spin $\frac{1}{2}$) we get the well known relation

$$k_F^3 = 3\pi^2 n . \tag{2.68}$$

2.6 Free bosons case

For a gas of free bosons the Hamiltonian is

$$H = \sum_q \omega_q\left(b^\dagger_q b_q + \frac{1}{2}\right) \tag{2.69}$$

where the creation/annihilation operators are related to the field operator by

$$\begin{aligned}\phi(x) &= \int\frac{d^3q}{(2\pi)^3}\phi_q e^{iqx} = \sqrt{\frac{\hbar}{2m\omega_q}}\int\frac{d^3q}{(2\pi)^3}\left(b_q+b^\dagger_{-q}\right)e^{iqx} \\ &= \sqrt{\frac{\hbar}{2m\omega_q}}\int\frac{d^3q}{(2\pi)^3}\left(b_q e^{iqx}+b^\dagger_q e^{-iqx}\right) .\end{aligned} \tag{2.70}$$

For bosons the ground state is the vacuum $|\phi\rangle = |0\rangle$, so when we take the expectation value to get the Green's function (which we call $D(x,t)$ in this case)

$$\begin{aligned} D(x-x',t) &= -i\langle 0|T\phi(x,t)\phi^\dagger(x',0)|0\rangle = \\ &= -i\left\{\langle 0|\phi(x,t)\phi^\dagger(x',0)\Theta(t) + \phi^\dagger(x',0)\phi(x,t)|0\rangle\Theta(-t)\right\} \end{aligned} \tag{2.71}$$

and substituting the Fourier transform 2.70

$$\begin{aligned} &= -i\frac{\hbar}{2m\omega_q}\int\frac{d^3q}{(2\pi)^3}\int\frac{d^3q'}{(2\pi)^3}\langle 0|\Big\{\left(b_q(t)+b^\dagger_{-q}(t)\right)\left(b^\dagger_{q'}+b_{-q'}\right)\Theta(t)+ \\ &\qquad + \left(b^\dagger_{q'}+b_{-q'}\right)\left(b_q(t)+b^\dagger_{-q}(t)\right)\Theta(-t)\Big\}|0\rangle e^{i(qx-q'x')} \\ &= -i\frac{\hbar}{2m\omega_q}\int\frac{d^3q}{(2\pi)^3}\langle 0|\Big\{b_q b_q^\dagger\Theta(t)e^{-i\omega_q t} + b_{-q}b^\dagger_{-q}\Theta(-t)e^{i\omega_q t}\Big\}|0\rangle e^{iq(x-x')} \\ &= \int\frac{d^3q}{(2\pi)^3}\underbrace{\left\{-i\frac{\hbar}{2m\omega_q}\left(\Theta(t)e^{-i\omega_q t}+\Theta(-t)e^{i\omega_q t}\right)\right\}}_{D(q,t)} e^{iq(x-x')}. \end{aligned} \tag{2.72}$$

We can get the propagator doing the last Fourier transform, as usual adding a regularization term with $\delta > 0$, so that we have

$$\begin{aligned} D(q,\nu) &= \frac{\hbar}{2mi\omega_q}\int_{-\infty}^{\infty} dt\left(\Theta(t)e^{-i\omega_q t}+\Theta(-t)e^{i\omega_q t}\right)e^{i\nu t-\delta|t|} \\ &= \frac{\hbar}{2mi\omega_q}\left(\int_0^\infty dt\, e^{i(\nu-\omega_q+i\delta)t} + \int_{-\infty}^0 dt\, e^{i(\nu+\omega_q-i\delta)t}\right) \\ &= \frac{\hbar}{2m\omega_q}\left(\underbrace{\frac{1}{\nu-(\omega_q-i\delta)}}_{\text{Emission}} + \underbrace{\frac{1}{-\nu-(\omega_q-i\delta)}}_{\text{Absorption}}\right) \end{aligned} \tag{2.73}$$

where we see that the propagator is made up of two terms: the forward time propagator which we call the *emission* term and has a pole in $\nu = \omega_q - i\delta$ and a backward time propagator which we call the *absorption* term and has a pole in $\nu = -\omega_q + i\delta$.

2.7 Adiabatic ignition of a potential - GML Theorem

Let's examine the case of of a potential

$$H(t) = H_0 + \lambda(t)V\,, \qquad \lambda(t) = e^{-\epsilon|t|} \tag{2.74}$$

so that $\tau_A = \epsilon^{-1}$. At $t = -\infty$ the ground state of the system, which we call $|-\infty\rangle$, is the same as the ground state of H_0 and if we evolve in the Heisenberg picture, it doesn't change in time (like all states in the Heisenberg picture). Now, remembering that the Scattering matrix is

$$S(t,-t) = U(t)U^\dagger(-t) \qquad \text{with } U(t) = e^{iH_0 t}e^{-iHt} \tag{2.75}$$

we can write the scattering matrix in the interval $(-\infty, t)$ as just

$$S(t,-\infty) = U(t). \tag{2.76}$$

Notice that $|-\infty\rangle$ is an interesting state, its evolution in the interaction picture is

$$|\psi_I(t)\rangle = e^{iH_0t}|\psi_S(t)\rangle = e^{iH_0t}e^{-iHt}|-\infty\rangle = U(t)|-\infty\rangle. \tag{2.77}$$

(remember that $|-\infty\rangle$ it's in the Heisenberg picture!). Also, the time evolution of operators in the Heisenberg representation is

$$\begin{aligned} A_H(t) &= e^{iHt}e^{-iH_0t}e^{iH_0t}Ae^{-iH_0t}e^{iH_0t}e^{-iHt} \\ &= e^{iHt}e^{-iH_0t}A_I(t)e^{iH_0t}e^{-iHt} \\ &= U^\dagger(t)A_I(t)U(t) \end{aligned} \tag{2.78}$$

so we can write the expectation value of a bunch of time ordered operators (at times $t_1 > t_2 > ... > t_r$) as

$$\begin{aligned} &\langle\psi|A(t_1)B(t_2)...R(t_r)|\psi\rangle_H = \\ &= \langle-\infty|\underbrace{U^\dagger(t_1)}_{S^\dagger(t_1,-\infty)}A_I(t_1)\underbrace{U(t_1)U^\dagger(t_2)}_{S(t_1,t_2)}B_I(t_2)U(t_2)...\underbrace{U(t_{r-1})U^\dagger(t_r)}_{S(t_{r-1},t_r)}R_I(t_r)\underbrace{U(t_r)}_{S(t_r,-\infty)}|-\infty\rangle \\ &= \langle-\infty|S^\dagger(t_1,-\infty)A_I(t_1)S(t_1,t_2)B_I(t_2)...S(t_{r-1},t_r)R_I(t_r)S(t_r,-\infty)|-\infty\rangle. \end{aligned} \tag{2.79}$$

Now we can get the state at $t = \infty$ via the Scattering matrix

$$\begin{aligned} S(\infty,t_1)S(t_1,-\infty)|-\infty\rangle &= |+\infty\rangle \\ \underbrace{S^\dagger(\infty,t_1)S(\infty,t_1)}_{\mathbb{1}}S(t_1,-\infty)|-\infty\rangle &= S^\dagger(\infty,t_1)|+\infty\rangle \end{aligned} \tag{2.80}$$

so taking the hermitian conjugate

$$\langle-\infty|S^\dagger(t_1,-\infty) = \langle+\infty|S(\infty,t_1) \tag{2.81}$$

which we can put into 2.79 to get

$$\begin{aligned} &\langle\psi|A(t_1)B(t_2)...R(t_r)|\psi\rangle_H = \\ &\quad= \langle+\infty|S(\infty,t_1)A_I(t_1)S(t_1,t_2)B_I(t_2)...S(t_{r-1},t_r)R_I(t_r)S(t_r,-\infty)|-\infty\rangle \end{aligned} \tag{2.82}$$

and we can write this one as the time ordered version of

$$\begin{aligned} &= \langle+\infty|T[S(\infty,t_1)...S(t_r,-\infty)A_I(t_1)B_I(t_2)...R_I(t_r)]|-\infty\rangle \\ &= \langle+\infty|T[S(\infty,-\infty)A_I(t_1)B_I(t_2)...R_I(t_r)]|-\infty\rangle. \end{aligned} \tag{2.83}$$

This was the most delicate step of the calculation: to see why the sign remains the same when we introduce the time ordering, we need to think back about S as a product of two U operators, then we can commute for free every operator $R_I(t_r)$ with $U(t_r)$ since they are at the same time. The right hand side of 2.82 then becomes

$$\langle+\infty|U^\dagger(t_1)U(t_1)A_I(t_1)U^\dagger(t_2)U(t_2)B_I(t_2)...U^\dagger(t_r)U(t_r)R_I(t_r)|-\infty\rangle \tag{2.84}$$

from this one we see that to take all the U's to the left, it takes an even number of transpositions: two for $U^\dagger(t_2)U(t_2)$, four for $U^\dagger(t_3)U(t_3)$, six for $U^\dagger(t_4)U(t_4)$, ecc... so even for fermions the sign in front of 2.83 is a plus. We obtain the (almost final) result

$$\langle\psi|A(t_1)B(t_2)...R(t_r)|\psi\rangle_H = \langle+\infty|T[S(\infty,-\infty)A_I(t_1)B_I(t_2)...R_I(t_r)]|-\infty\rangle \tag{2.85}$$

If the adiabatic principle really holds, then the final state $|+\infty\rangle$ is the same as the starting one $|-\infty\rangle$. It is usually a convention to call this phase $e^{2i\delta}$, so that $|+\infty\rangle = e^{2i\delta}|-\infty\rangle$ or

$$\langle+\infty| = e^{-2i\delta}\langle-\infty| = \frac{\langle-\infty|}{\langle-\infty|\infty\rangle} = \frac{\langle-\infty|}{\langle-\infty|S[\infty,-\infty]|-\infty\rangle} \tag{2.86}$$

and inserting this expression into 2.85 we finally get the *Gell-Man and Low theorem*

$$\langle\psi|T[A(t_1)B(t_2)...R(t_r)]|\psi\rangle_H = \frac{\langle-\infty|T[S(\infty,-\infty)A(t_1)B(t_2)...R(t_r)]|-\infty\rangle}{\langle-\infty|S[\infty,-\infty]|-\infty\rangle} \tag{2.87}$$

where we have put the time ordering also in the left hand side since it was our first assumption that the operators were time ordered.

2.8 Spectral representation of the propagator

We define the spectral function

$$A(k,\omega) = \frac{1}{\pi}\mathrm{Im}\left\{G(k,\omega - i\delta)\right\} \tag{2.88}$$

now using Cauchy's principal value equation

$$\frac{1}{\omega - i\delta} = P\left(\frac{1}{\omega}\right) + i\pi\delta(\omega) \tag{2.89}$$

so that if we introduce the new *spectral representation* of the propagator

$$\begin{aligned}
G(k,\omega) &= \sum_\lambda \frac{|M_\lambda(k)|^2}{\omega - \epsilon_\lambda + i\delta_\lambda} \\
\rightarrow A(k,\omega) &= \sum_\lambda |M_\lambda(k)|^2\delta(\omega - \epsilon_\lambda) \\
&= \sum_\lambda \left[|\langle\lambda|c^\dagger_{k\sigma}|\phi\rangle|^2\theta(\omega) + |\langle\lambda|c_{k\sigma}|\phi\rangle|^2\theta(-\omega)\right]\delta(|\omega| - (E_\lambda - E_g)) \\
&= \theta(\omega)\rho_e(k,\omega) + \theta(-\omega)\rho_h(k,-\omega)
\end{aligned} \tag{2.90}$$

such that

$$\begin{aligned}
\rho_e(k,\omega) &= \sum_\lambda |\langle\lambda|c^\dagger_{k\sigma}|\phi\rangle|^2\delta(\omega - (E_\lambda - E_g)) \qquad (\omega > 0) \\
\rho_h(k,\omega) &= \sum_\lambda |\langle\lambda|c_{k\sigma}|\phi\rangle|^2\delta(\omega - (E_g - E_\lambda)) \qquad (\omega > 0)
\end{aligned} \tag{2.91}$$

Now we can expand the Green's function as follows

$$
\begin{aligned}
G(k,t) &= -i\langle\phi|c_{k\sigma}(t)c^{\dagger}_{k\sigma}(0)\theta(t) - c^{\dagger}_{k\sigma}(0)c_{k\sigma}(t)\theta(-t)|\phi\rangle \\
&= -i\sum_{\lambda}\Big\{\langle\phi|c_{k\sigma}(t)|\lambda\rangle\langle\lambda|c^{\dagger}_{k\sigma}(0)|\phi\rangle\theta(t) - \langle\phi|c^{\dagger}_{k\sigma}(0)|\lambda\rangle\langle\lambda|c_{k\sigma}(t)|\phi\rangle\theta(-t)\Big\} \\
&= -i\sum_{\lambda}\Big\{\langle\phi|e^{iHt}c_{k\sigma}e^{-iHt}|\lambda\rangle\langle\lambda|c^{\dagger}_{k\sigma}|\phi\rangle\theta(t) - \langle\phi|c^{\dagger}_{k\sigma}|\lambda\rangle\langle\lambda|e^{iHt}c_{k\sigma}e^{-iHt}|\phi\rangle\theta(-t)\Big\} \\
&= -i\sum_{\lambda}\Big\{|\langle\lambda|c^{\dagger}_{k\sigma}|\phi\rangle|^2 e^{i(E_g-E_\lambda)t}\theta(t) - |\langle\lambda|c_{k\sigma}|\phi\rangle|^2 e^{i(E_\lambda-E_g)t}\theta(-t)\Big\}
\end{aligned}
\tag{2.92}
$$

so now Fourier transforming and introducing the regularization term δ

$$
G(k,\omega) = \sum_{\lambda}\left\{\frac{|\langle\lambda|c^{\dagger}_{k\sigma}|\phi\rangle|^2}{\omega-(E_\lambda-E_g)+i\delta} + \frac{|\langle\lambda|c_{k\sigma}|\phi\rangle|^2}{\omega-(E_g-E_\lambda)-i\delta}\right\} \tag{2.93}
$$

3 Assignment 1

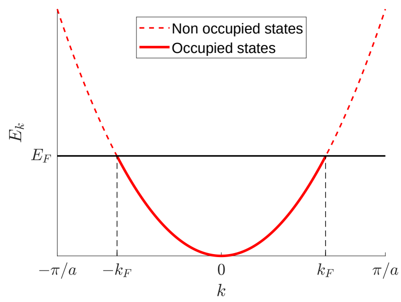
3.1 Pauli exclusion in metals

One dimensional gas of free electrons at temperature $T = 0$.

a) The system is described by the Hamiltonian

$$\hat{H}_0 = \frac{L}{2\pi}\int dk \sum_{\sigma} E_k \hat{c}^{\dagger}_{k\sigma}\hat{c}_{k\sigma}\,, \tag{3.1}$$

$$E_k = \frac{\hbar k^2}{2m_*} \tag{3.2}$$



at $T = 0$ the Fermi-Dirac distribution can be approximated by a step function, such that the occupation number is 1 up to the *Fermi energy* $E_F = \frac{\hbar^2 k_F^2}{2m_*}$ and 0 for bigger energies. We can then write the ground state as

$$|\phi\rangle = \prod_{|k|<k_F,\sigma} \hat{c}^{\dagger}_{k}|0\rangle \tag{3.3}$$

b) The total number of electrons is

$$\begin{aligned} N = \langle\phi|\hat{N}|\phi\rangle &= \frac{L}{2\pi}\int dk \sum_{\sigma}\langle\phi|\hat{c}^{\dagger}_{k\sigma}\hat{c}_{k\sigma}|\phi\rangle \\ &= \frac{L}{2\pi}2\int_{-\infty}^{\infty} dk\,\Theta(k_F - |k|) = \frac{L}{\pi}2k_F \end{aligned} \tag{3.4}$$

$$\rightarrow \bar{n} = \frac{2}{\pi}k_F \tag{3.5}$$

c) Consider the spin-resolved density-density correlation function

$$\begin{aligned} C^{(0)}_{\sigma,\sigma'}(x) &= \langle\hat{\rho}_{\sigma}(x)\hat{\rho}_{\sigma'}(0)\rangle_0 = \langle\phi|\hat{\psi}^{\dagger}_{\sigma}(x)\hat{\psi}_{\sigma}(x)\hat{\psi}^{\dagger}_{\sigma'}(0)\hat{\psi}_{\sigma'}(0)|\phi\rangle \\ &= \underbrace{\langle\phi|\hat{\psi}^{\dagger}_{\sigma}(x)\hat{\psi}_{\sigma'}(0)|\phi\rangle}_{A} - \underbrace{\langle\phi|\hat{\psi}^{\dagger}_{\sigma}(x)\hat{\psi}^{\dagger}_{\sigma'}(0)\hat{\psi}_{\sigma}(x)\hat{\psi}_{\sigma'}(0)|\phi\rangle}_{B} \end{aligned} \tag{3.6}$$

having commuted the two fermionic operators in the middle. The first term can be different than zero only for $\sigma = \sigma'$ and $x = 0$, then it becomes half the average density (just half since it's not summed on the spin as before)

$$A = \delta_{\sigma\sigma'}\delta(x)\langle\phi|\hat{\psi}^{\dagger}_{\sigma}(x)\hat{\psi}_{\sigma}(x)|\phi\rangle = \delta_{\sigma\sigma'}\delta(x)\frac{\bar{n}}{2}. \tag{3.7}$$

The second term can be rewritten as a Green's function if we include an infinitesimal time delay

$$\begin{aligned} B = \langle\phi|\hat{\psi}^\dagger_\sigma(x,0^+)\hat{\psi}^\dagger_{\sigma'}(0,0+)\hat{\psi}_\sigma(x,0)\hat{\psi}_{\sigma'}(0,0)|\phi\rangle = \\ = (-1)^6\langle\phi|T[\hat{\psi}_\sigma(x,0)\hat{\psi}_{\sigma'}(0,0)\hat{\psi}^\dagger_{\sigma'}(0,0+)\hat{\psi}^\dagger_\sigma(x,0^+)]|\phi\rangle \\ = -G(1,2;1',2') \end{aligned} \tag{3.8}$$

$$\text{where} \quad \begin{aligned} 1 &= (x,0,\sigma)\,, & 2 &= (0,0,\sigma')\,, \\ 1' &= (x,0^+,\sigma)\,, & 2' &= (0,0^+,\sigma')\,. \end{aligned} \tag{3.9}$$

Now, using Wick's theorem and the Green's function for fermions we found at lecture

$$\begin{aligned} B &= -G(1,1')G(2,2') + G(1,2')G(2,1') \\ &= -[G(0,0^-)]^2 + \delta_{\sigma\sigma'}G(x,0^-)G(-x,0^-) \end{aligned} \tag{3.10}$$

$$G(0,0^-) = \frac{i}{2\pi}\int_{-\infty}^{\infty} dk\Theta(k_F - |k|) = i\frac{k_F}{\pi} = i\frac{\bar{n}}{2} \tag{3.11}$$

$$G(x,0^-) = \frac{i}{2\pi}\int_{-\infty}^{\infty} dk\Theta(k_F - |k|)e^{-ikx} = i\frac{sin(k_F x)}{\pi x} = i\frac{\bar{n}}{2}\frac{sin(k_F x)}{k_F x} \tag{3.12}$$

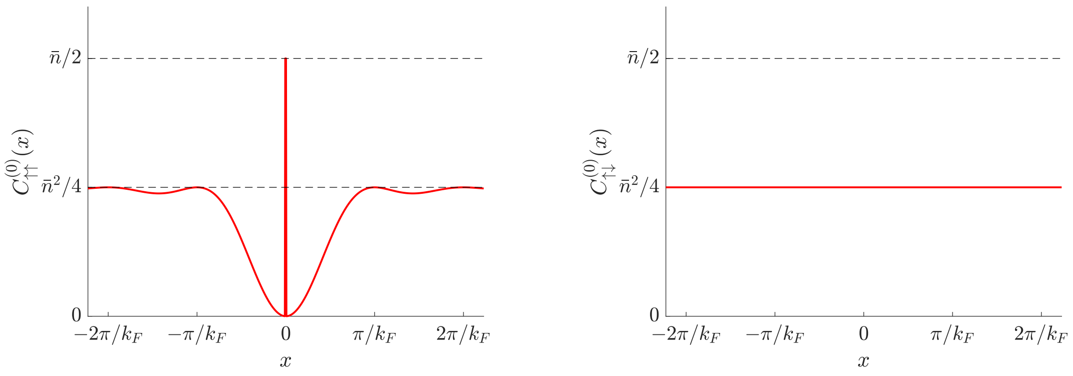
so that putting all together

$$C^{(0)}_{\sigma,\sigma'}(x) = \delta_{\sigma\sigma'}\delta(x)\frac{\bar{n}}{2} + \frac{\bar{n}^2}{4} - \delta_{\sigma\sigma'}\frac{\bar{n}^2}{4}\frac{sin^2(k_F x)}{(k_F x)^2} \tag{3.13}$$

d) Using $\hat{\rho}(x) = \hat{\rho}_\uparrow(x) + \hat{\rho}_\downarrow(x)$

$$\begin{aligned} C^{(0)}(x) &= \langle[\hat{\rho}_\uparrow(x) + \hat{\rho}_\downarrow(x)][\hat{\rho}_\uparrow(0)\hat{\rho}_\downarrow(0)]\rangle_0 = \sum_{\sigma,\sigma'} C^{(0)}_{\sigma,\sigma'}(x) \\ &= \delta(x)\bar{n} + \bar{n}^2 - \frac{\bar{n}^2}{2}\frac{sin^2(k_F x)}{(k_F x)^2} \\ &= \bar{n}\left[\delta(x) + \bar{n}\underbrace{\left(1 - \frac{1}{2}\frac{sin^2(k_F x)}{(k_F x)^2}\right)}_{g_0(x)}\right] \end{aligned} \tag{3.14}$$

Below are sketched the functions $C^{(0)}_{\uparrow\uparrow}(x)$, $C^{(0)}_{\uparrow\downarrow}(x)$ and $g_0(x)$.



(a) (b)

Figure 2: Density-density correlation as a function of the position: (a) for same-spin electrons, (b) for opposite-spin electrons.

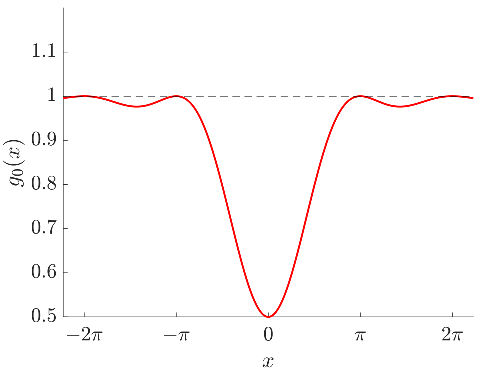


Figure 3: Function $g_0(x)$ that appears in equation 3.14. The local maxima are in multiples of π.

e) Pauli exclusion principle would be valid for two particles in the *same* position (and same spin), but given Heisenberg uncertainty principle the position of a particle is not exactly defined and we find that the Pauli repulsion is somehow valid in a range of positions Δx. As we can see from the figure 2a, $\Delta x \sim 2\pi/k_F$.

3.2 Hartree-Fock

The full Hamiltonian is

$$H = \sum_\sigma \int d^3r\, \hat{\psi}^\dagger_\sigma(r) \left[-\frac{\hbar^2}{2m}\nabla^2 + V_0(r) \right] \hat{\psi}_\sigma(r) + \frac{1}{2}\sum_{\sigma\sigma'} \int d^3r \int d^3r'\, V_{ee}(r-r')\hat{\psi}^\dagger_{\sigma'}(r')\hat{\psi}^\dagger_\sigma(r)\hat{\psi}_\sigma(r)\hat{\psi}_{\sigma'}(r') \tag{3.15}$$

with the trial state being

$$|\psi_{MF}\rangle = \prod_{\alpha=1}^{N} \hat{d}_\alpha^\dagger |0\rangle. \tag{3.16}$$

a) Let's first look at how to change basis from the field operators to the $\hat{d}$ ones

$$\begin{aligned}
\hat{\psi}_\sigma(r) &= \sum_\alpha \langle r,\sigma|\alpha\rangle \hat{d}_\alpha = \sum_\alpha \varphi_\alpha(r,\sigma)\hat{d}_\alpha \\
\hat{\psi}_\sigma^\dagger(r) &= \sum_\alpha \langle \alpha|r,\sigma\rangle \hat{d}_\alpha^\dagger = \sum_\alpha \varphi_\alpha^*(r,\sigma)\hat{d}_\alpha^\dagger
\end{aligned} \tag{3.17}$$

Substituting these into the Hamiltonian we get

$$\begin{aligned}
H = &\sum_{\alpha\beta}\sum_\sigma \int d^3r\, \varphi_\alpha^*(r,\sigma)\left[-\frac{\hbar^2}{2m}\nabla^2 + V_0(r)\right]\varphi_\beta(r,\sigma)\hat{d}_\alpha^\dagger \hat{d}_\beta \\
&+ \frac{1}{2}\sum_{\alpha\alpha'\beta\beta'}\sum_{\sigma\sigma'}\int d^3r \int d^3r'\, V_{ee}(r-r')\varphi_{\alpha'}^*(r',\sigma')\varphi_\alpha^*(r,\sigma)\varphi_\beta(r,\sigma)\varphi_{\beta'}(r',\sigma')\hat{d}_{\alpha'}^\dagger \hat{d}_\alpha^\dagger \hat{d}_\beta \hat{d}_{\beta'}\,.
\end{aligned} \tag{3.18}$$

The calculation of $E_{MF} = \langle\psi_{MF}|H|\psi_{MF}\rangle$ is somewhat similar to the one we already did in the first exercise, taking the expectation value of the first term onto the trial state

$$\langle\psi_{MF}|H_0|\psi_{MF}\rangle = \sum_{\alpha\leq N}\sum_\sigma \int d^3r\, \varphi_\alpha^*(r,\sigma)\left[-\frac{\hbar^2}{2m}\nabla^2 + V_0(r)\right]\varphi_\alpha(r,\sigma) \tag{3.19}$$

where we are constrained by the fact that only the occupied states can be annihilated by $\hat{d}_\beta$ **and** the selection rules allow only the diagonal terms to survive. Taking the expectation value of the second term of 3.18 and using Wick's theorem

$$\begin{aligned}
&\frac{1}{2}\sum_{\alpha\alpha'\beta\beta'}\sum_{\sigma\sigma'}\int d^3r\, d^3r'\, V_{ee}(r-r')\varphi_{\alpha'}^*(r',\sigma')\varphi_\alpha^*(r,\sigma)\varphi_\beta(r,\sigma)\varphi_{\beta'}(r',\sigma')\langle\psi_{MF}|\hat{d}_{\alpha'}^\dagger \hat{d}_\alpha^\dagger \hat{d}_\beta \hat{d}_{\beta'}|\psi_{MF}\rangle \\
=&\frac{1}{2}\sum_{\substack{\alpha,\alpha'\\ \beta,\beta'\leq N}}\sum_{\sigma\sigma'}\int d^3r\, d^3r'\, V_{ee}(r-r')\varphi_{\alpha'}^*(r',\sigma')\varphi_\alpha^*(r,\sigma)\varphi_\beta(r,\sigma)\varphi_{\beta'}(r',\sigma')\Big(\delta_{\alpha\beta}\delta_{\alpha'\beta'} - \delta_{\alpha'\beta}\delta_{\alpha\beta'}\Big) \\
=&\frac{1}{2}\sum_{\alpha,\alpha'\leq N}\sum_{\sigma\sigma'}\int d^3r\, d^3r'\, V_{ee}(r-r')\Big[|\varphi_\alpha(r,\sigma)|^2|\varphi_{\alpha'}(r',\sigma')|^2 - \varphi_{\alpha'}^*(r',\sigma')\varphi_{\alpha'}(r,\sigma)\varphi_\alpha^*(r,\sigma)\varphi_\alpha(r',\sigma')\Big]
\end{aligned} \tag{3.20}$$

b-c) We define the functional

$$F = E_{MF} - \sum_{\alpha'\leq N}\int d^3r'\, \epsilon_{\alpha'}\left(\sum_{\sigma'}|\varphi_{\alpha'}(r',\sigma')|^2 - 1\right) \tag{3.21}$$

such that minimizing it with respect to $\varphi^*_\alpha(r,\sigma)$ we get[4]

$$\frac{\delta F}{\delta\varphi^*_\alpha(r,\sigma)} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_0(r)\right)\varphi_\alpha(r,\sigma) + \overbrace{\sum_{\alpha'\leq N}\sum_{\sigma'}\int d^3r'\,V_{ee}(r-r')|\varphi_{\alpha'}(r',\sigma')|^2}^{V_H(r)}\,\varphi_\alpha(r,\sigma)$$
$$-\sum_{\sigma'}\int d^3r'\,\underbrace{\sum_{\alpha'\leq N} V_{ee}(r-r')\varphi^*_{\alpha'}(r',\sigma')\varphi_{\alpha'}(r,\sigma)}_{[V_F]_{\sigma\sigma'}(r,r')}\,\varphi_\alpha(r',\sigma') - \epsilon_\alpha\varphi_\alpha(r,\sigma) = 0 \tag{3.22}$$

$$\to \left(-\frac{\hbar^2}{2m}\nabla^2 + V_0(r) + V_H(r)\right)\varphi_\alpha(r,\sigma) - \sum_{\sigma'}\int d^3r'\,[V_F]_{\sigma\sigma'}(r,r')\varphi_\alpha(r',\sigma') = \epsilon_\alpha\varphi_\alpha(r,\sigma) \tag{3.23}$$

and minimizing with respect to $\varphi_\alpha(r,\sigma)$ we would just get the complex conjugate of this equation.

d) Looking for a moment at the so called *Hartree potential*, we can move the summation signs to make it look like

$$V_H(r) = \int d^3r' V_{ee}(r-r')\underbrace{\sum_{\alpha'\leq N}\sum_{\sigma'}|\varphi_{\alpha'}(r',\sigma')|^2}_{\rho(r')} = \int d^3r' V_{ee}(r-r')\rho(r') \tag{3.24}$$

so what we're doing is averaging all the orbitals into a single potential. In our approximation, if we try to put a new electron in the system it will be interacting with this *mean* potential, instead of having two particle interactions with all the other electrons.

e) In equation 3.23, if we multiply both sides by $\varphi^*_\alpha(r,\sigma)$ and then sum on α, σ and integrate on r, on the right hand side we get

$$\sum_{\alpha\leq N}\epsilon_\alpha \underbrace{\sum_\sigma\int d^3r\,\varphi^*_\alpha(r,\sigma)\varphi_\alpha(r,\sigma)}_{=1} = \sum_{\alpha\leq N}\epsilon_\alpha \tag{3.25}$$

while on the left hand side

$$\sum_{\alpha\leq N}\sum_\sigma\int d^3r\,\varphi^*_\alpha(r,\sigma)\Big[\left(-\frac{\hbar^2}{2m}\nabla^2 + V_0(r) + V_H(r)\right)\varphi_\alpha(r,\sigma)$$
$$-\sum_{\sigma'}\int d^3r'[V_F]_{\sigma\sigma'}(r,r')\varphi_\alpha(r',\sigma')\Big]. \tag{3.26}$$

[4] The $\frac{1}{2}$ goes away from the interaction terms because they contain two φ^*, so that taking a functional derivative gives two terms, where the second one is just the same as the first one but with a different choice of variable names. Since those variables are summed/integrated out, we can just rename them to make it look the same as the first (this property is the analogue of what $\partial_x x^2 = 2x$ is for normal derivatives).

We can rewrite E_{MF} with the *Hartree* and *Fock* potentials

$$E_{MF} = \sum_{\alpha\leq N}\sum_{\sigma}\int d^3r\,\varphi_\alpha^*(r,\sigma)\Big[\left(-\frac{\hbar^2}{2m}\nabla^2 + V_0(r) + \frac{1}{2}V_H(r)\right)\varphi_\alpha(r,\sigma) \\ -\frac{1}{2}\sum_{\sigma'}\int d^3r'[V_F]_{\sigma\sigma'}(r,r')\varphi_\alpha(r',\sigma')\Big] \tag{3.27}$$

to see that the difference $E_{\rm crxn} = \sum_{\alpha\leq N}\epsilon_\alpha - E_{MF}$ is just

$$E_{\rm crxn} = \frac{1}{2}\sum_{\alpha\leq N}\sum_{\sigma}\int d^3r\,\varphi_\alpha^*(r,\sigma)\Big[V_H(r)\varphi_\alpha(r,\sigma) - \sum_{\sigma'}\int d^3r'[V_F]_{\sigma\sigma'}(r,r')\varphi_\alpha(r',\sigma')\Big]. \tag{3.28}$$

4 Assignment 2

4.1 Expansion of S matrix to second order

a) The S matrix operator can be written as a perturbative series, which cut at second order looks like

$$\hat{S}(\infty,-\infty) = \mathbb{1} - \frac{i}{\hbar}\int_{-\infty}^{\infty} dt_1 \hat{V}(t_1) - \frac{1}{2\hbar^2}\int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2\, T\{\hat{V}(t_1)\hat{V}(t_2)\} + O(V^3) \quad (4.1)$$

so that when it's evaluated on the ground state I call each term

$$\langle\phi_0|\hat{S}(\infty,-\infty)|\phi_0\rangle = 1 + S_0^{(1)} + S_0^{(2)} + O(V^3). \quad (4.2)$$

In the case of a 2-body potential

$$\hat{V}(t_1) = \frac{1}{2}\int dx_1 \int dx_2 \int dt_2\, \hat{\psi}^\dagger(x_1)\hat{\psi}^\dagger(x_2)\underbrace{V(x_1-x_2)\delta(t_1-t_2)}_{V(1,2)}\hat{\psi}(x_2)\hat{\psi}(x_1) \quad (4.3)$$

the second order of the S matrix expansion is

$$\begin{aligned}
S_0^{(2)} &= -\frac{1}{8\hbar^2}\int d1\, d2\, d3\, d4\, V(1,2)V(3,4)\langle\varphi_0|T\{\hat{\psi}^\dagger(1)\hat{\psi}^\dagger(2)\hat{\psi}(2)\hat{\psi}(1)\hat{\psi}^\dagger(3)\hat{\psi}^\dagger(4)\hat{\psi}(4)\hat{\psi}(3)\}|\varphi_0\rangle \\
&= -\frac{(-1)^8}{8\hbar^2}\int d1\, d2\, d3\, d4\, V(1,2)V(3,4)\langle\varphi_0|T\{\hat{\psi}(4)\hat{\psi}(3)\hat{\psi}(2)\hat{\psi}(1)\hat{\psi}^\dagger(1)\hat{\psi}^\dagger(2)\hat{\psi}^\dagger(3)\hat{\psi}^\dagger(4)\}|\varphi_0\rangle \\
&= -\frac{1}{8\hbar^2}\int d1\, d2\, d3\, d4\, V(1,2)V(3,4)(i)^4 G^0(1,2,3,4;4,3,2,1) \\
&= -\frac{1}{8\hbar^2}\int d1\, d2\, d3\, d4\, V(1,2)V(3,4)\begin{vmatrix} G(1,1) & G(1,2) & G(1,3) & G(1,4) \\ G(2,1) & G(2,2) & G(2,3) & G(2,4) \\ G(3,1) & G(3,1) & G(3,3) & G(3,4) \\ G(4,1) & G(4,2) & G(4,3) & G(4,4) \end{vmatrix} \\
&= -\frac{1}{8\hbar^2}\int d1\, d2\, d3\, d4\, \{\text{diagrams in figure 4}\}
\end{aligned} \quad (4.4)$$

b) The diagram in the blue rectangle in figure 4 is given by a product of two potentials and four Green's functions. Inserting the Fourier transform of each of them we get

$$\begin{aligned}
&G(1,1)V(1,2)G(2,3)G(3,4)V(3,4)G(4,2) = \\
&= \int_{k_1,\omega_1} G(k_1,\omega_1)e^{i\omega 0^+}\int_{q_1} V(q_1)e^{iq_1(x_1-x_2)}\int_{k_2,\omega_2} G(k_2,\omega_2)e^{ik_2(x_2-x_3)}e^{-i\omega_2(t_2-t_3)}\times \\
&\times \int_{k_3,\omega_3} G(k_3,\omega_3)e^{ik_3(x_3-x_4)}e^{-i\omega_3(t_3-t_4)}\int_{q_2} V(q_2)e^{iq_2(x_3-x_4)}\int_{k_4,\omega_4} G(k_4,\omega_4)e^{ik_4(x_4-x_2)} \\
&\qquad e^{-i\omega_4(t_4-t_2)}
\end{aligned} \quad (4.5)$$

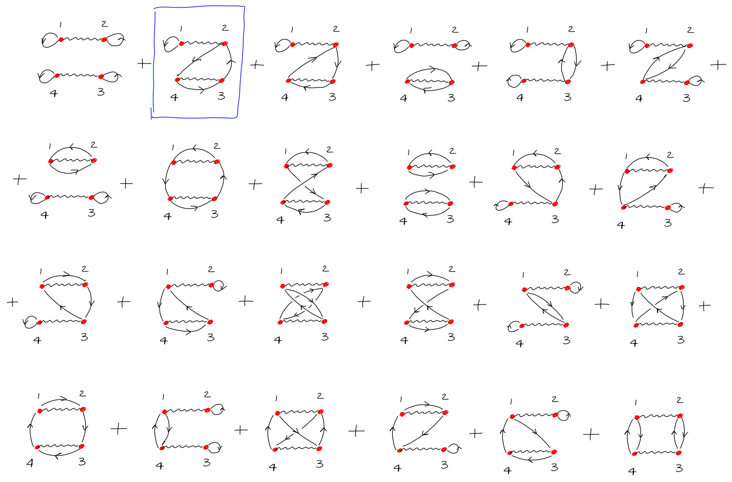


Figure 4: All the possible diagrams that can come out of equation 4.4. The one in a blue rectangle is the one I've chosen for questions **b** and **c**.

now integrating over $d1\, d2\, d3\, d4$ as in equation 4.4 we get some delta functions which enforce momentum and energy conservation

$$\begin{gathered}\delta(q_1)\delta(k_2 - k_4 - q_1)\delta(k_3 + q_2 - k_2)\delta(k_4 - q_2 - k_3)\times \\ \times\delta(\omega_2 - \omega_4)\delta(\omega_3 - \omega_2)\delta(\omega_4 - \omega_3)\end{gathered} \tag{4.6}$$

so we get to the final expression

$$\int_{k_1,\omega_1,k_2,\omega_2,q_1,q_2} V(q_1)\delta(q_1)V(q_2)G(k_1,\omega_1)G(k_2,\omega_2)G(k_2-q_2,\omega_2)G(k_2-q_1,\omega_2) \tag{4.7}$$

which corresponds to the momentum space diagram in figure 5.

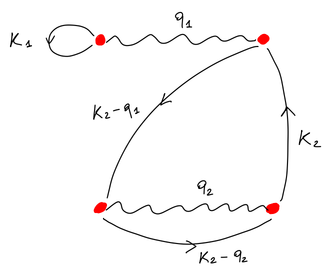


Figure 5: Diagram in momentum space corresponding to 4.7.

c) Given the diagram selected in figure 4, we name every line (propagator) with a different momentum variables k_1, k_2, k_3, k_4 and the two interaction lines with q_1, q_2. Enforcing conservation of energy and momentum at every vertex (same as the deltas in 4.6) we recover the same expression as 4.7. Now in the last section we had a pre factor of $-\frac{1}{8}$, but there were 8 topologically equivalent diagrams so this class of diagrams had a -1 in front.

We recover the same here given that there are two interactions so we get a $(-i)^2$ plus the symmetry factor is 1 because every permutation of the vertices would change the relative orientation of the arrows.

d) In figure 6 there are 3 examples of disconnected diagrams and 3 examples of connected diagrams that would come out at second order expanding the expression

$$\langle\varphi_0|T\{\hat{S}\hat{\psi}(1)\hat{\psi}^\dagger(2)\}|\varphi_0\rangle \tag{4.8}$$

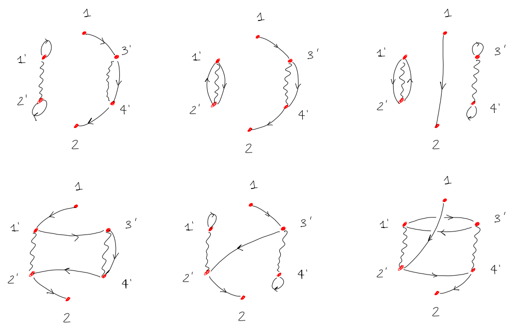


Figure 6: Example of disconnected and connected diagrams that could arise from expanding expression 4.8 at second order.

4.2 Green's functions in the presence of an impurity potential

One dimensional metal at temperature T, the electrons are free but there is an impurity potential

$$\hat{H} = \hat{H}_0 + \hat{V} \tag{4.9}$$

$$\hat{H}_0 = \sum_k \xi_k \hat{c}_k^\dagger \hat{c}_k \,, \quad \xi_k = \frac{\hbar^2 k^2}{2m} - \mu \tag{4.10}$$

$$\hat{V} = \int dx\, \alpha\delta(x-x_0)\hat{\psi}^\dagger(x)\hat{\psi}(x) \tag{4.11}$$

the Green's function for the complete Hamiltonian is

$$G_{kk'}(\tau-\tau') = -\big\langle T_\tau[\hat{c}_k(\tau)\hat{c}_{k'}^\dagger(\tau')]\big\rangle = -\frac{\big\langle T_\tau[\hat{S}_I(\beta,0)\hat{c}_{I,k}(\tau)\hat{c}_{I,k'}^\dagger(\tau')]\big\rangle_0}{\big\langle \hat{S}_I(\beta,0)\big\rangle_0} \tag{4.12}$$

a) Inserting the Fourier transform of the field operators we can get the alternative expression for the potential

$$\begin{aligned}
\hat{V} &= \int dx\, \alpha\delta(x-x_0)\sum_{k_2}\hat{c}_{k_2}^\dagger e^{-ik_2x}\sum_{k_1}\hat{c}_{k_1}e^{ik_1x} \\
&= \frac{\alpha}{V}\int dx \sum_{k_1k_2} V\delta(x-x_0)e^{-i(k_2-k_1)x}\hat{c}_{k_2}^\dagger\hat{c}_{k_1} \\
&= \frac{\alpha}{V}\sum_{k_1k_2} e^{-i(k_2-k_1)x_0}\hat{c}_{k_2}^\dagger\hat{c}_{k_1}
\end{aligned} \tag{4.13}$$

b) Evaluating the denominator of 4.12 at first order

$$\langle \hat{S}_I(\beta,0)\rangle_0 = 1 - \int_0^\beta d\tau_1 \langle \hat{V}_I(\tau_1)\rangle_0 \tag{4.14}$$

so using the expression found in the last paragraph we get

$$\begin{aligned}\langle \hat{S}_I(\beta,0)\rangle_0 &= 1 - \frac{\alpha}{V}\int_0^\beta d\tau_1 \sum_k \langle \hat{c}_k^\dagger(\tau_1)\hat{c}_k(\tau_1)\rangle_0 \\ &= 1 + \frac{\alpha}{V}\int_0^\beta d\tau_1 \sum_k \langle T[\hat{c}_k(\tau_1)\hat{c}_k^\dagger(\tau_1^+)]\rangle_0 \\ &= 1 - \frac{\alpha\beta}{V}\sum_k G_k^0(0^-)\end{aligned} \tag{4.15}$$

and now we can insert the Matsubara Fourier transform of the Green's function

$$\begin{aligned}\langle \hat{S}_I(\beta,0)\rangle_0 = 1 - \frac{\alpha\beta}{V}\sum_{k,i\omega_n} G_k^0(i\omega_n)e^{i\omega_n 0^+} &= 1 - \frac{\alpha\beta}{V}\sum_k \int \frac{dz}{2\pi i}\frac{e^{z0^+}}{z-\xi_k}f(z) \\ = 1 - \frac{\alpha\beta}{V}\sum_k f(\xi_k) = 1 - \alpha\beta n_0 &\end{aligned} \tag{4.16}$$

having used Cauchy's theorem and having called $f(\xi)$ the Fermi-Dirac distribution.

c) Looking now at the numerator of 4.12 and doing the same expansion at first order

$$\begin{aligned}&\langle T_\tau[\hat{S}_I(\beta,0)\hat{c}_{I,k}(\tau)\hat{c}^\dagger_{I,k'}(\tau')]\rangle_0 = \langle T_\tau[\Big\{\mathbb{1} - \int_0^\beta d\tau_1 \hat{V}_I(\tau_1)\Big\}\hat{c}_{I,k}(\tau)\hat{c}^\dagger_{I,k'}(\tau')]\rangle_0 \\ &= \langle T_\tau[\hat{c}_{I,k}(\tau)\hat{c}^\dagger_{I,k'}(\tau')]\rangle_0 - \frac{\alpha}{V}\int_0^\beta d\tau_1 \sum_{k_1k_2} e^{-i(k_2-k_1)x_0}\langle T_\tau[\hat{c}^\dagger_{I,k_2}(\tau_1^+)\hat{c}_{I,k_1}(\tau_1)\hat{c}_{I,k}(\tau)\hat{c}^\dagger_{I,k'}(\tau')]\rangle_0\end{aligned} \tag{4.17}$$

where the first term is just

$$\langle T_\tau[\hat{c}_{I,k}(\tau)\hat{c}^\dagger_{I,k'}(\tau')]\rangle_0 = -G^0_{kk'}(\tau-\tau') = -\delta_{kk'}G^0_k(\tau-\tau') \tag{4.18}$$

and the second term becomes, using Wick's theorem

$$\begin{aligned}&\frac{\alpha}{V}\int_0^\beta d\tau_1 \sum_{k_1k_2} e^{-i(k_2-k_1)x_0} G^0\Big((k_1,\tau_1),(k,\tau);(k',\tau'),(k_2,\tau_1^+)\Big) \\ &= \frac{\alpha}{V}\int_0^\beta d\tau_1 \sum_{k_1k_2} e^{-i(k_2-k_1)x_0}\Big[G^0_{k_1k_2}(\tau_1-\tau_1^+)G^0_{kk'}(\tau-\tau') - G^0_{k_1k'}(\tau_1-\tau')G^0_{kk_2}(\tau-\tau_1^+)\Big] \\ &= \frac{\alpha}{V}\int_0^\beta d\tau_1 \Big[\underbrace{\sum_{k_1} G^0_{k_1}(0^-)}_{Vn_0}\delta_{kk'}G^0_k(\tau-\tau') - e^{-i(k-k')x_0}G^0_{k'}(\tau_1-\tau')G^0_k(\tau-\tau_1)\Big] \\ &= \alpha\beta n_0\,\delta_{kk'}G^0_k(\tau-\tau') - \frac{\alpha}{V}e^{-i(k-k')x_0}[G^0_k * G^0_{k'}](\tau-\tau')\end{aligned} \tag{4.19}$$

so in total the numerator is (keeping in mind there was a minus in front)

$$\mathcal{N} = \delta_{kk'} G^0_k(\tau - \tau')\big(1 - \alpha\beta n_0\big) + \frac{\alpha}{V} e^{-i(k-k')x_0} [G^0_k * G^0_{k'}](\tau - \tau') \tag{4.20}$$

d) Now we want to evaluate the ratio $\mathcal{N}/(1-\alpha\beta n_0)$, but for small α we can Taylor expand at first order, so that

$$\begin{aligned} \frac{\mathcal{N}}{(1-\alpha\beta n_0)} &\simeq \mathcal{N}\big(1 + \alpha\beta n_0 + O(\alpha^2)\big) \\ \to G_{kk'}(\tau - \tau') &\simeq \delta_{kk'} G^0_k(\tau - \tau') + \frac{\alpha}{V} e^{-i(k-k')x_0} [G^0_k * G^0_{k'}](\tau - \tau') + O(\alpha^2) \end{aligned} \tag{4.21}$$

e) Our end goal is to Fourier transform the last equation on both sides. Lets look at how the two convoluted Green's functions transform to Matsubara frequency space

$$\begin{aligned} [G^0_k * G^0_{k'}](\tau - \tau') &= \int_0^\beta d\tau_1\, G^0_k(\tau - \tau_1) G^0_{k'}(\tau_1 - \tau') \\ &= \int_0^\beta d\tau_1\, \frac{1}{\beta}\sum_n G^0_k(i\omega_n) e^{-i\omega_n(\tau-\tau_1)} \frac{1}{\beta}\sum_m G^0_{k'}(i\omega'_m) e^{-i\omega'_m(\tau_1-\tau')} \\ &= \frac{1}{\beta^2}\sum_{nm} G^0_k(i\omega_n) e^{-i\omega_n\tau} G^0_{k'}(i\omega'_m) e^{i\omega'_m\tau'} \underbrace{\int_0^\beta d\tau_1\, e^{-i(\omega'_m-\omega_n)\tau_1}}_{\beta\,\delta_{\omega'_m\omega_n}} \\ &= \frac{1}{\beta}\sum_n G^0_k(i\omega_n) G^0_{k'}(i\omega_n) e^{-i\omega_n(\tau-\tau')} \end{aligned} \tag{4.22}$$

f) Now we can finally Fourier transform both sides of 4.21

$$\begin{aligned} \frac{1}{\beta}\sum_n G_{kk'}(i\omega_n) e^{-i\omega_n(\tau-\tau')} = \frac{1}{\beta}\sum_n \Big\{ &\delta_{kk'} G_k(i\omega_n) \\ &+ \frac{\alpha}{V} e^{-i(k-k')x_0} G_k(i\omega_n) G_{k'}(i\omega_n) \Big\} e^{-i\omega_n(\tau-\tau')} \end{aligned} \tag{4.23}$$

so that at first order in α the complete Green's function is

$$G_{kk'}(i\omega_n) = \delta_{kk'} G_k(i\omega_n) + \frac{\alpha}{V} e^{-i(k-k')x_0} G_k(i\omega_n) G_{k'}(i\omega_n) \tag{4.24}$$

and substituting the free Green's function for fermions

$$G_{kk'}(i\omega_n) = \frac{\delta_{kk'}}{i\omega_n - \xi_k} + \frac{\alpha}{V} \frac{e^{-i(k-k')x_0}}{(i\omega_n - \xi_k)(i\omega_n - \xi_{k'})} \tag{4.25}$$

g) By analytical continuation $i\omega_n \to \omega + i\delta$, we find the retarded Green's function

$$G^R_{kk'}(i\omega_n) = \frac{\delta_{kk'}}{\omega - \xi_k + i\delta} + \frac{\alpha}{V} \frac{e^{-i(k-k')x_0}}{(\omega - \xi_k + i\delta)(\omega - \xi_{k'} + i\delta)} \tag{4.26}$$

4.3 Polarization function for non-interacting electrons

a) The imaginary-time response function is

$$\begin{aligned}\chi_0(\mathbf{q},\tau) &= -\frac{1}{V}\langle T_\tau[\hat{\rho}(\mathbf{q},\tau)\hat{\rho}(-\mathbf{q},0)]\rangle \\ &= -\frac{1}{V}\sum_{\mathbf{k}\mathbf{k}'\sigma\sigma'}\langle T_\tau[\hat{c}^\dagger_{\mathbf{k}\sigma}(\tau)\hat{c}_{\mathbf{k}+\mathbf{q}\sigma}(\tau)\hat{c}^\dagger_{\mathbf{k}'\sigma'}(0)\hat{c}_{\mathbf{k}'-\mathbf{q}\sigma'}(0)]\rangle\end{aligned} \tag{4.27}$$

since we're in the non-interacting case we can use Wick's theorem

$$\chi_0(\mathbf{q},\tau) = -\frac{1}{V}\sum_{\mathbf{k}\mathbf{k}'\sigma\sigma'}\Big[\delta_{\mathbf{q}0}G^0_{\mathbf{k}\sigma}(0^-)G^0_{\mathbf{k}'\sigma'}(0^-) - \delta_{\mathbf{k}+\mathbf{q},\mathbf{k}'}\delta_{\sigma\sigma'}G^0_{\mathbf{k}'\sigma'}(\tau)G^0_{\mathbf{k}\sigma}(-\tau)\Big] \tag{4.28}$$

so if $\mathbf{q} \neq 0$ we can keep only the second term

$$\chi_0(\mathbf{q},\tau) = \frac{1}{V}\sum_{\mathbf{k}\sigma}G^0_{\mathbf{k}+\mathbf{q}\sigma}(\tau)G^0_{\mathbf{k}\sigma}(-\tau) \tag{4.29}$$

b) Now we can insert the Matsubara frequency Fourier transform of the Green's functions

$$\chi_0(\mathbf{q},\tau) = \frac{1}{V}\sum_{\mathbf{k}\sigma}\frac{1}{\beta^2}\sum_{i\omega_l}G^0_{\mathbf{k}+\mathbf{q}\sigma}(i\omega_l)e^{-i\omega_l\tau}\sum_{ik_m}G^0_{\mathbf{k}\sigma}(ik_m)e^{-ik_m(-\tau)} \tag{4.30}$$

so the Matsubara frequency response function is

$$\begin{aligned}\chi_0(\mathbf{q},iq_n) &= \int_0^\beta d\tau\chi_0(\mathbf{q},\tau)e^{iq_n\tau} \\ &= \frac{1}{V\beta^2}\sum_{\mathbf{k}\sigma}\sum_{i\omega_l,ik_m}G^0_{\mathbf{k}+\mathbf{q}\sigma}(i\omega_l)G^0_{\mathbf{k}\sigma}(ik_m)\overbrace{\int_0^\beta d\tau e^{-i(\omega_l-k_m-q_n)\tau}}^{\beta\,\delta_{\omega_l,k_m+q_n}} \\ &= \frac{1}{V\beta}\sum_{\mathbf{k}\sigma}\sum_{ik_m}G^0_{\mathbf{k}+\mathbf{q}\sigma}(ik_m+iq_n)G^0_{\mathbf{k}\sigma}(ik_m) \\ &= \frac{1}{V\beta}\sum_{\mathbf{k}\sigma}\sum_{ik_m}\frac{1}{(i(k_m+q_n)-\xi_{\mathbf{k}+\mathbf{q}})(ik_m-\xi_{\mathbf{k}})}\end{aligned} \tag{4.31}$$

which by Cauchy's integral theorem and taking an appropriate contour C can be written as

$$\chi_0(\mathbf{q},iq_n) = \frac{1}{V}\sum_{\mathbf{k}\sigma}\oint_C\frac{dz}{2\pi i}\frac{f(z)}{(z+iq_n-\xi_{\mathbf{k}+\mathbf{q}})(z-\xi_{\mathbf{k}})} \tag{4.32}$$

with $f(z)$ being the analytical continuation of the Fermi-Dirac distribution to the whole complex plane. Since f is exponential in the real line, it is periodic though the imaginary one with the Matsubara frequencies as a period. We can now use residues' theorem to write the integral as a sum of the two residues over the two poles $z = \xi_{\mathbf{k}}$ and $z = \xi_{\mathbf{k}+\mathbf{q}} - iq_n$

$$\begin{aligned}\chi_0(\mathbf{q},iq_n) &= \frac{1}{V}\sum_{\mathbf{k}\sigma}\Big(\frac{f(\xi_{\mathbf{k}})}{iq_n-\xi_{\mathbf{k}+\mathbf{q}}+\xi_{\mathbf{k}}} + \frac{f(\xi_{\mathbf{k}+\mathbf{q}}-iq_n)}{\xi_{\mathbf{k}+\mathbf{q}}-iq_n-\xi_{\mathbf{k}}}\Big) \\ &= \frac{2}{V}\sum_{\mathbf{k}}\frac{f(\xi_{\mathbf{k}})-f(\xi_{\mathbf{k}+\mathbf{q}})}{iq_n-\xi_{\mathbf{k}+\mathbf{q}}+\xi_{\mathbf{k}}}\end{aligned} \tag{4.33}$$

c) Now we can perform the analytical continuation $iq_n \to \omega + i\delta$ to recover the retarded response function

$$\chi_0^R(\mathbf{q}, \omega) = \frac{2}{V} \sum_{\mathbf{k}} \frac{f(\xi_{\mathbf{k}}) - f(\xi_{\mathbf{k}+\mathbf{q}})}{\omega - (\xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}}) + i\delta} \tag{4.34}$$