MASTER'S DEGREE IN PHYSICS
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Introduction to Many Body Theory

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HOMEWORK 2

First Exercise

To compute the Green function for a non interacting homogeneous system we must start from the general expression for the green function of an homogeneous system:

$$G_{\alpha\beta}(\mathbf{k},\omega) = \hbar V \sum_n \left[\frac{\langle\phi_0|\hat{\psi}_\alpha(0)|n,\mathbf{k}\rangle\ \langle n,\mathbf{k}|\hat{\psi}^\dagger_\beta(0)|\phi_0\rangle}{\hbar\omega - \mu - \mathcal{E}^{(N+1)}_{\mathbf{k}} + i\eta} + \frac{\langle\phi_0|\hat{\psi}^\dagger_\beta(0)|n,-\mathbf{k}\rangle\ \langle n,-\mathbf{k}|\hat{\psi}_\alpha(0)|\phi_0\rangle}{\hbar\omega - \mu - \mathcal{E}^{(N-1)}_{\mathbf{k}} - i\eta} \right] \quad (1)$$

where the fields are defined in terms of the single particle wavefunctions $\varphi_{\mathbf{k}}(\mathbf{x})$ as follows:

$$\hat{\psi}_\alpha(0) = \sum_{\mathbf{k}'} \varphi_{\mathbf{k}'}(0)\hat{c}_{\mathbf{k}',\alpha} \qquad \hat{\psi}^\dagger_\beta(0) = \sum_{\mathbf{k}''} \varphi_{\mathbf{k}''}(0)\hat{c}^\dagger_{\mathbf{k}',\alpha}. \quad (2)$$

We notice that for a non interacting system a complete set of eigenstates for the momentum operator $\hat{\vec{P}}$ is also a complete set of eigenstates for the Hamiltonian $\hat{H}$; the excited states of the system are identified just by the $\mathbf{k}$ index and thus the sum over n in (1) is unnecessary and can be omitted.
Let's proceed computing the matrix elements in (1). The first semplification of the expression is given by the dyad $|\mathbf{k}\rangle\langle\mathbf{k}|$, which "selects" in the summations over $\mathbf{k}'$ and $\mathbf{k}''$, introduced by the definitions of the fields, the only terms with momentum equal to $\mathbf{k}$:

$$\begin{aligned}
\langle\phi_0|\hat{\psi}_\alpha(0)|\mathbf{k}\rangle\ \langle\mathbf{k}|\hat{\psi}^\dagger_\beta(0)|\phi_0\rangle &= \sum_{\mathbf{k}'\mathbf{k}''} \langle\phi_0|\varphi_{\mathbf{k}'}(0)\hat{c}_{\mathbf{k}',\alpha}|\mathbf{k}\rangle\ \langle\mathbf{k}|\varphi^\dagger_{\mathbf{k}''}(0)\hat{c}^\dagger_{\mathbf{k}'',\beta}|\phi_0\rangle\,\Theta(k-k_F) &(3)\\
&= \sum_{\mathbf{k}',\mathbf{k}''} \varphi_{\mathbf{k}'}(0)\varphi^\dagger_{\mathbf{k}''}(0)\,\langle\mathbf{k}',\alpha|\mathbf{k}\rangle\ \langle\mathbf{k}|\mathbf{k}'',\beta\rangle\,\Theta(k-k_F) &(4)\\
&= \sum_{\mathbf{k}',\mathbf{k}''} \varphi_{\mathbf{k}'}(0)\varphi^\dagger_{\mathbf{k}''}(0)\delta_{\alpha,\beta}\delta_{\mathbf{k}',\mathbf{k}}\delta_{\mathbf{k}'',\mathbf{k}}\Theta(k-k_F) &(5)\\
&= |\varphi_{\mathbf{k}}(0)|^2\delta_{\alpha,\beta}\Theta(k-k_F). &(6)
\end{aligned}$$

In (3) we introduced the $\Theta(k-k_F)$: this is due to the fact that the field operators are acting in both the matrix elements as creation operators over a filled Fermi sphere: in this situation all contributions to the sum like $\hat{c}^\dagger_{\mathbf{k}}|\phi_0\rangle$ for $k<k_F$ are annihilated due to the exclusion principle. The second couple of matrix elements in (1) is computed similarly:

$$\langle\phi_0|\hat{\psi}^\dagger_\beta(0)|n,-\mathbf{k}\rangle\ \langle n,-\mathbf{k}|\hat{\psi}_\alpha(0)|\phi_0\rangle = |\varphi_{-\mathbf{k}}(0)|^2\delta_{\alpha,\beta}\Theta(k_F-k); \quad (7)$$

in this case the limitation to the sum is applied to all the values of k above the Fermi level, since the ladder operators act in both the matrix element as destruction operators on the ground state $|\phi_0\rangle$.

The denominators both contain an addend which is the excitation energy of the system with $N+1$ particles ($N-1$ respectively). This term can be rewtitten as a function of the momentum k, since in a non interacting system it indicizes the excited states:

$$\begin{aligned}
\mathcal{E}^{(N+1)}_{\mathbf{k}} &= E^{(N+1)}_{\mathbf{k}} - E^{(N+1)} &(8)\\
&= E^{(N+1)}_{\mathbf{k}} - E^{(N)} - \left(E^{(N+1)} - E^{(N)}\right) &(9)\\
&= \mathcal{E}^0_{\mathbf{k}} - \mathcal{E}^0_F &(10)\\
&= \frac{\hbar^2}{2m}\left(k^2 - k_F^2\right) &(11)
\end{aligned}$$

and similarly for the $\mathcal{E}_{-\mathbf{k}}^{(N-1)}$ term:

$$\mathcal{E}_{-\mathbf{k}}^{(N-1)} = \frac{\hbar^2}{2m}\big(k_F^2 - k^2\big). \tag{12}$$

The chemical potential μ is assumed equal for the $N \to N+1$ and $N \to N-1$ excitations:

$$\mu = E^{(N+1)} - E^{(N)} = E^{(N-1)} - E^{(N)} = \frac{\hbar^2 k_F^2}{2m} \tag{13}$$

Substituting the epressions (11) and (13) in the first denominator of (1) one finds

$$\hbar\omega - mu - \mathcal{E}_k^{(N+1)} + i\eta \;=\; \hbar\omega - \frac{\hbar^2 k_F^2}{2m} - \frac{\hbar^2}{2m}\big(k^2 - k_F^2\big) + i\eta \;=\; \hbar(\omega - \omega_k) + i\eta. \tag{14}$$

The derivation for the other denominator is equivalent.

Gathering the results together, one finds the Green function for an homogeneous non interacting system:

$$iG^0_{\alpha,\beta}(\mathbf{k},\omega) = V|\varphi_{\mathbf{k}}(0)|^2 \left[\frac{\Theta(k-k_F)}{\omega-\omega_k+i\eta} + \frac{\Theta(k_F-k)}{\omega-\omega_k-i\eta}\right]\delta_{\alpha,\beta}. \tag{15}$$

In the last expression we canceled out the $\hbar$ factors, redefining $\hbar\eta \to \eta$, since it is a quantity tending to zero and its value is not relevant for the calculation. In the special case of electrons, which we described as plane waves

$$\varphi_{\mathbf{k}}(\mathbf{x}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{x}} \tag{16}$$

the prefactor $|\varphi_{\mathbf{k}}(0)|^2$ reads:

$$|\varphi_{\mathbf{k}}(0)|^2 = V^{-1} \tag{17}$$

and this leads us to the well known expression for the Green function of a non interacting system of electrons:

$$iG^0_{\alpha,\beta}(\mathbf{k},\omega) = \delta_{\alpha,\beta}\left[\frac{\Theta(k-k_F)}{\omega-\omega_k+i\eta} + \frac{\Theta(k_F-k)}{\omega-\omega_k-i\eta}\right]. \tag{18}$$

1 Second Exercise

In the following steps we are going to compute the mean value of the total number operator $\hat{N}$ and the total energy E_0 of an non interacting system of electrons.

The density for a generic operator $\hat{J}$ in second quantization is expressed as a function of the first quantized operator $J_{\alpha,\beta}$

$$\hat{j}(\mathbf{x}) = \hat{\psi}^\dagger_\beta(\mathbf{x}) J_{\beta\alpha}(\mathbf{x}) \hat{\psi}_\alpha(\mathbf{x}); \tag{19}$$

given this expression the mean value of the $\hat{j}(\mathbf{x})$ operator density over the ground state $|\psi_0\rangle$ can be expressed as:

$$\langle\psi_0|\hat{j}(\mathbf{x})|\psi_0\rangle = \pm i \lim_{\substack{\mathbf{x}'\to\mathbf{x} \\ t'\to t^+}} \mathrm{Tr}\left[J(\mathbf{x})G(\mathbf{x},t,\mathbf{x}',t')\right] \tag{20}$$

where the $'+'$ is for bosons and the $'-'$ for fermions.

The total number operator density is:

$$\hat{N} = \int \mathrm{d}\mathbf{x}\, n(\mathbf{x}); \qquad\qquad \hat{n}(\mathbf{x}) = \hat{\psi}^\dagger_\beta(\mathbf{x}) \delta_{\beta\alpha} \hat{\psi}_\alpha(\mathbf{x}) \tag{21}$$

and thus we can compute its mean value for a non interacting system of electrons using (20):

$$\langle\psi_0|\hat{n}(\mathbf{x})|\psi_0\rangle = -i \lim_{\substack{\mathbf{x}'\to\mathbf{x} \\ t'\to t^+}} \sum_{\alpha,\beta} \delta_{\alpha\beta} G^0_{\beta\alpha}(\mathbf{x},t,\mathbf{x}',t') \tag{22}$$

$$= -i \lim_{\substack{\mathbf{x}'\to\mathbf{x} \\ t'\to t^+}} \sum_{\alpha,\beta} \delta_{\alpha\beta}\delta_{\beta\alpha} \frac{1}{V} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} e^{-i\omega_k(t-t')} \times \tag{23}$$

$$\times \left[\Theta(t-t')\Theta(k-k_F) - \Theta(t'-t)\Theta(k_F-k)\right]. \tag{24}$$

Performing the time limit the term relative to $\Theta(t-t')$ vanishes and the time dependent exponential is evaluated to one; applying the constraint on the $\mathbf{k}$ sum given by $\Theta(k_F - k)$ we can write:

$$\langle\psi_0|\hat{n}(\mathbf{x})|\psi_0\rangle = \frac{1}{V} \lim_{\mathbf{x}'\to\mathbf{x}} \sum_{\alpha,\beta} \delta_{\alpha\beta}\delta_{\beta\alpha} \sum_{|\mathbf{k}|<k_F} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \tag{25}$$

which, performing the final spatial limit, becomes:

$$\langle\psi_0|\hat{n}(\mathbf{x})|\psi_0\rangle = \frac{1}{V} \sum_{\alpha,\beta} \delta_{\alpha\beta}\delta_{\beta\alpha} \sum_{|\mathbf{k}|<k_F} 1. \tag{26}$$

An integration over $\mathbf{x}$ allows us to pass from the mean value of $\hat{n}(\mathbf{x})$ to the one of $\hat{N}$:

$$\langle\psi_0|\hat{N}|\psi_0\rangle = \int \mathrm{d}^3\mathbf{x}\, \frac{1}{V} \sum_{\alpha,\beta} \delta_{\alpha\beta}\delta_{\beta\alpha} \sum_{|\mathbf{k}|<k_F} 1 \tag{27}$$

$$= \sum_{\alpha,\beta} \delta_{\alpha\beta}\delta_{\beta\alpha} \sum_{|\mathbf{k}|<k_F} 1 \tag{28}$$

The remaining sum over $\mathbf{k}$ is none but the number N of $\mathbf{k}$ states inside the Fermi sphere, while the sum over α and β is the trace of the identity of the spin space, namely the spin space dimension, which is equal to $2s + 1$ for half-integer values. The mean value of the number operator $\hat{N}$ for a non interacting system of electrons is then:

$$\langle\psi_0|\hat{N}|\psi_0\rangle = 2N. \tag{29}$$

To compute the total ground state energy E_0 of a non interacting system of electrons it is sufficient to compute the kinetic contribution $\hat{T}$ to the Hamiltonian $\hat{H} = \hat{T} + \hat{V}$ since the interaction potential is null by definition. The mean value of the $\hat{T}$ operator is defined as

$$\langle\psi_0|\hat{T}|\psi_0\rangle = -i \int \mathrm{d}^3\mathbf{x} \lim_{\substack{\mathbf{x}'\to\mathbf{x} \\ t'\to t^+}} -\frac{\hbar^2\nabla^2}{2m} \sum_{\alpha,\beta} \delta_{\alpha\beta} G^0_{\beta\alpha}(\mathbf{x},t,\mathbf{x}',t') \tag{30}$$

which, in the special case of a non interacting system of electrons, becomes:

$$\langle\psi_0|\hat{T}|\psi_0\rangle = \frac{1}{V}\sum_{\alpha,\beta}\delta_{\alpha\beta}\delta_{\beta\alpha}\int \mathrm{d}^3\mathbf{x} \lim_{\substack{\mathbf{x}'\to\mathbf{x}\\ t'\to t^+}} \frac{\hbar^2\nabla^2}{2m}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}e^{-i\omega_k(t-t')}\times \tag{31}$$

$$\times\left[\Theta(t-t')\Theta(k-k_F)-\Theta(t'-t)\Theta(k_F-k)\right] \tag{32}$$

$$= -\frac{2s+1}{V}\int \mathrm{d}^3\mathbf{x} \lim_{\mathbf{x}'\to\mathbf{x}} \frac{\hbar^2\nabla^2}{2m}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}\Theta(k_F-k) \tag{33}$$

$$= +\frac{2s+1}{V}\int \mathrm{d}^3\mathbf{x} \lim_{\mathbf{x}'\to\mathbf{x}} \sum_{\mathbf{k}} \frac{\hbar^2\mathbf{k}^2}{2m} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}\Theta(k_F-k) \tag{34}$$

$$= \frac{2s+1}{V}\sum_{|\mathbf{k}|<k_F}\frac{\hbar^2\mathbf{k}^2}{2m}\int \mathrm{d}^3\mathbf{x}\,\underbrace{\lim_{\mathbf{x}'\to\mathbf{x}} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}}_{\to 1} \tag{35}$$

$$= (2s+1)\sum_{|\mathbf{k}|<k_F}\frac{\hbar^2\mathbf{k}^2}{2m}. \tag{36}$$

Substituting the spin value $s = 1/2$ of the electrons we obtain in the end:

$$E_0 = 2\sum_{|\mathbf{k}|<k_F}\frac{\hbar^2\mathbf{k}^2}{2m}. \tag{37}$$