Problem set 5

1. A many-electron system is described by the Hamiltonian

$$\mathcal{H} = \sum_\sigma \int d\vec{r}\Psi_\sigma^\dagger(\vec{r})\left(-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right)\Psi_\sigma(\vec{r}) + \frac{1}{2}\sum_{\sigma,\sigma'}\int d\vec{r}d\vec{r}'\Psi_\sigma^\dagger(\vec{r})\Psi_{\sigma'}^\dagger(\vec{r}')V(\vec{r}-\vec{r}')\Psi_{\sigma'}(\vec{r}')\Psi_\sigma(\vec{r})$$

where the field operators obey the anticommutation relations $\left\{\Psi_\sigma(\vec{r}), \Psi_{\sigma'}^\dagger(\vec{r}')\right\} = \delta(\vec{r}-\vec{r}')$ and $\{\Psi, \Psi\} = \left\{\Psi^\dagger, \Psi^\dagger\right\} = 0$.

(a) Starting from the definition of the zero-temperature causal Green's function, derive its equation of motion $i\hbar\partial G_{\sigma\sigma'}(\vec{r}t, \vec{r}'t')/\partial t = ...$ Some hints are given in the class notes, however you should write down the full derivation.

(b) express the expectation value of the potential energy in terms of the causal two-particle Green's function, using the tricks we employed for expectation values of one-particle operators (set $t' = t + \eta$, where $\eta \to 0$ is a small positive number, for the $\Psi^\dagger$ field operators, etc).

(c) combine results from (a) and (b) to obtain the general expression for the total ground-state energy of the system, both in real space-time, and for the Fourier transform. (The final equations are listed at the bottom of page 7 and on page 8 of the notes).

(d) Use the last formula (page 8 of the notes) for the free electrons causal Green's function and show that you obtain the correct ground-state energy. What would happen if you took the limit $\eta \to 0$ before carrying out the frequency integral?

2. Assume a homogeneous, interacting N-particle system. In this case, we expect the momenta to be good quantum numbers, and we can expand the field operators $\Psi_\sigma(\vec{r}) = \sum_{\vec{k}} \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}} c_{\vec{k}\sigma}$, etc. Find the general expressions of $G_{\sigma\sigma'}(\vec{k}, t, t')$, $G_{\sigma\sigma'}^{R/A}(\vec{k}, t, t')$ where $G_{\sigma\sigma'}(\vec{k}, t, t') = \int d\vec{r}e^{-i\vec{k}\cdot\vec{r}}G_{\sigma\sigma'}(\vec{r}t, \vec{0}t')$, etc, in terms of ground-state expectation values involving the $c_{k\sigma,H}(t), c_{k\sigma,H}^\dagger(t)$ operators. What is the physical meaning of this causal Green's function?

b) we define the **spectral function** as $A_{\sigma\sigma'}(\vec{k}, \omega) = i[G_{\sigma\sigma'}^R(\vec{k}, \omega) - G_{\sigma\sigma'}^A(\vec{k}, \omega)]$. Show that:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_{\sigma\sigma'}(\vec{k}, \omega) = \delta_{\sigma\sigma'}$$

c) For free fermions, $\mathcal{H} = \sum_{\vec{k},\sigma} \epsilon_{\vec{k}} c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma}$, calculate $G_{\sigma\sigma'}^{R/A}(\vec{k}, \omega)$ explicitly. Check that the identity derived at (b) holds trivially in this case.

3. Consider a system with short-range electron-electron interactions described by $v(\vec{r}-\vec{r}') = V_0\delta(\vec{r}-\vec{r}')$.

(a) compute the proper self-energy in the Hartree-Fock approximation (i.e., keep only first-order diagrams in the proper self-energy expansion). Solve the Dyson equation to find out the Green's function in this approximation. From its poles, find out the excitation spectrum of the system, $E_{\vec{k}}$, if we assume that the dispersion of non-interacting electrons is described by $\epsilon_{\vec{k}} = \hbar^2k^2/2m$.

(b) Use the self-consistent Hartree-Fock equations we derived using the variational approach to check the result you found at (a). You can start directly from any equations derived in the notes.

(c) Draw all second-order diagrams that contribute to $\Sigma^*(\vec{k}, \omega)$. Point out which ones have a trivial (i.e., no) dependence on $(\vec{k}, \omega)$, and therefore will just shift the total energy, without changing the dispersion of the quasiparticles. Pick one of the remaining non-trivial diagrams and compute its expression.

4. Let's have some real fun now, with electron-phonon interactions. Consider the Hamiltonian:

$$\mathcal{H} = \sum_{k,\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_q \hbar\Omega_q b^\dagger_q b_q + \sum_{k,q,\sigma} g_{k,q} c^\dagger_{k-q,\sigma} c_{k\sigma} \left(b^\dagger_q + b_{-q} \right)$$

Derive diagrammatics rules for $G_{\sigma,\sigma'}(k,\omega)$ (the Fourier transform of the one-particle, causal Green's function).

Pointers:

a) the division into $H_0 = \sum_{k,\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_q \hbar\Omega_q b^\dagger_q b_q$ and $H_1 = \sum_{k,q,\sigma} g_{k,q} c^\dagger_{k-q,\sigma} c_{k\sigma} \left(b^\dagger_q + b_{-q} \right)$ should be obvious.

b) sketch the main points on how one gets to express $G_{\sigma,\sigma'}(k,t,t')$ as a ratio of two series, each of which contains expectations values over the non-interacting ground-state $|\phi_0\rangle$. Is there any difference with respect to the notes (excepting the obviously different type of interaction?). What is the non-interacting, N-electron ground state $|\phi_0\rangle$?

c) now consider the first few orders in the series for both $g^{(n)}_{\sigma\sigma'}(k,t,t')$ and $s^{(n)}$. I know I haven't given you a Wick's theorem for bosons, but for the lowest orders you can easily calculate the expectation values for bosons by hand. Note: the last problem from the previous set should suggest to you that you may see $D_0(k,t,t')$ appear for the phonons (these will be the contractions of the bosonic operators, basically). Invent some diagrammatic rules. It's easier working in (k,ω) space, so Fourier transform everything.

d) argue that Bruecker theorem holds, and that only connected diagrams contribute to $G_{\sigma,\sigma'}(k,\omega)$. What is the expression of the proper self-energy?

e) optional: one could similarly derive diagramatics to find the change in the phonon propagator, $D(k,\omega)$ as compared to the non-interacting one. Think about how you would do this, and what would be the lowest order contributions.