Problem Set 6
Quantum Field Theory and Many Body Physics (SoSe2015)

Due: Tuesday, May 26, 2015 with Yang Peng

In this problem set, we study some aspects of Green functions and their equations of motion. In the first problem, we show that for interacting systems, equations of motion for the Green functions involve more complicated Green functions whose equations of motion involve yet more complicated Green functions etc. In the second problem, we write down explicit Lehmann-like representations for the single-particle Green functions of non-interacting systems and use these important expressions to give an alternative derivation of the polarization operator from the equation of motion. Finally, the third problem continues with interacting systems and discusses how the infinite hierarchy of equations of motion can be truncated to yield important approximation schemes. Specifically, we discuss how the Hartree-Fock approximation looks in the equations of motion approach.

Problem 1: Equations of motion for the field operators (5+5+5+10 points)

In this problem, we derive the Heisenberg equation of motion of the field operator

$$\psi(\mathbf{r},t) = e^{iHt}\psi(\mathbf{r})e^{-iHt} \tag{1}$$

for a Hamiltonian of the form

$$H = \int d\mathbf{r}\, \psi^\dagger(\mathbf{r}) \left(-\frac{\nabla^2}{2m} + U(\mathbf{r})\right) \psi(\mathbf{r}) + \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}')v(\mathbf{r}-\mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r}). \tag{2}$$

We will consider both bosons and fermions.

(a) Using the relation (prove!)

$$[A, BC] = [A, B]_\pm C \mp B[A, C]_\pm, \tag{3}$$

evaluate the commutator in the Heisenberg equation of motion

$$i\frac{\partial\psi}{\partial t} = [\psi, H] \tag{4}$$

to find

$$i\frac{\partial\psi(\mathbf{r},t)}{\partial t} = \left(-\frac{\nabla^2}{2m} + U(\mathbf{r})\right)\psi(\mathbf{r},t) + \int d\mathbf{r}' v(\mathbf{r}-\mathbf{r}')\psi^\dagger(\mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r}). \tag{5}$$

Write down the analogous equation for $\psi^\dagger(\mathbf{r},t)$.

(b) Solve this equation of motion explicitly for free particles [i.e., for $v(\mathbf{r}-\mathbf{r}') = 0$] with single-particle spectrum

$$\left(-\frac{\nabla^2}{2m} + U(\mathbf{r})\right)\varphi_\alpha(\mathbf{r}) = \epsilon_\alpha\varphi_\alpha(\mathbf{r}). \tag{6}$$

To do so, expand

$$\psi(\mathbf{r},t) = \sum_\alpha \varphi_\alpha(\mathbf{r})c_\alpha(t) \tag{7}$$

and show that

$$c_\alpha(t) = e^{-i\epsilon_\alpha t}c_\alpha, \tag{8}$$

where c_α is the Schrödinger operator.

(c) Find the corresponding results for the Heisenberg operator $\psi(\mathbf{r},\tau) = e^{H\tau}\psi(\mathbf{r})e^{-H\tau}$ in imaginary time.

(d) Use your result in (c) to write down an equation of motion for

$$\mathcal{G}(\mathbf{r}\tau,\mathbf{r}'\tau') = \langle \mathrm{T}_\tau \psi(\mathbf{r},\tau)\psi^\dagger(\mathbf{r}',\tau')\rangle, \tag{9}$$

i.e., compute $\partial_\tau \mathcal{G}(\mathbf{r}\tau,\mathbf{r}'\tau')$ as well as $\partial_{\tau'}\mathcal{G}(\mathbf{r}\tau,\mathbf{r}'\tau')$. Note that in the presence of a two-body interaction $v(\mathbf{r}-\mathbf{r}')$, the equation of motion includes higher-order correlation (or Green) functions of the type

$$\langle \mathrm{T}_\tau \psi(\mathbf{r}_1,\tau_1)\psi(\mathbf{r}_2,\tau_2)\psi^\dagger(\mathbf{r}_3,\tau_3)\psi^\dagger(\mathbf{r}_4,\tau_4)\rangle. \tag{10}$$

In principle, we can then derive equations of motion for these higher-order Green functions which will generate yet higher-order Green functions etc.

Problem 2: Free particle Green's functions (8+8+9 points)

In this problem, we derive explicit expressions for the single-particle Green functions and apply them to give another derivation of the polarization operator Π_0 which we discussed in a previous problem set.

(a) Compute the finite temperature Green functions

$$\begin{aligned}
G(\mathbf{r}t,\mathbf{r}'t') &= -i\langle \mathrm{T}\psi(\mathbf{r},t)\psi^\dagger(\mathbf{r}',t')\rangle, &(11)\\
G^R(\mathbf{r}t,\mathbf{r}'t') &= -i\,\theta(t-t')\langle[\psi(\mathbf{r},t),\psi^\dagger(\mathbf{r}',t')]_\mp\rangle, &(12)\\
G^A(\mathbf{r}t,\mathbf{r}'t') &= i\,\theta(t'-t)\langle[\psi(\mathbf{r},t),\psi^\dagger(\mathbf{r}',t')]_\mp\rangle, &(13)\\
\mathcal{G}(\mathbf{r}\tau,\mathbf{r}'\tau') &= \langle \mathrm{T}_\tau\psi(\mathbf{r},\tau)\psi^\dagger(\mathbf{r}',\tau')\rangle &(14)
\end{aligned}$$

in the time domain.

(b) Fourier transform the result to obtain

$$\begin{aligned}
G(\mathbf{r},r';\omega) &= \sum_\alpha \phi_\alpha(\mathbf{r})\phi_\alpha^*(\mathbf{r}')\left[\frac{1\pm n(\epsilon_\alpha)}{\omega-\epsilon_\alpha+i\eta}\mp\frac{n(\epsilon_\alpha)}{\omega-\epsilon_\alpha-i\eta}\right], &(15)\\
G^R(\mathbf{r},r';\omega) &= \sum_\alpha \frac{\phi_\alpha(\mathbf{r})\phi_\alpha^*(\mathbf{r}')}{\omega-\epsilon_\alpha+i\eta}, &(16)\\
G^A(\mathbf{r},r';\omega) &= \sum_\alpha \frac{\phi_\alpha(\mathbf{r})\phi_\alpha^*(\mathbf{r}')}{\omega-\epsilon_\alpha-i\eta}, &(17)\\
\mathcal{G}(\mathbf{r},r';i\omega_n) &= -\sum_\alpha \frac{\phi_\alpha(\mathbf{r})\phi_\alpha^*(\mathbf{r}')}{i\omega_n-\epsilon_\alpha}. &(18)
\end{aligned}$$

Note that for many body systems, it is more appropriate to consider the thermal averages $\langle\ldots\rangle$ as grand-canonical averages. This corresponds to the replacement $H\to H-\mu N$. This does not cause any changes if we agree to measure single particle energies from the chemical potential μ.

(c) Consider the equation of motion for a non-interacting system

$$[\partial_\tau + H_0 + U(\mathbf{r})]\mathcal{G}_0(\mathbf{r}\tau,\mathbf{r}'\tau') = \delta(\mathbf{r}-\mathbf{r}')\delta(\tau-\tau'), \tag{19}$$

in which we made the potential $U(\mathbf{r})$ explicit so that H_0 just contains the kinetic energy.[1] We now want to compute the Green function to linear order in this potential and use this to compute the change in density induced by $U(\mathbf{r})$. This is just what is described by the polarization operator which we discussed in a previous problem set. First show that the (number) density can be expressed as

$$n(\mathbf{r},\tau) = \pm\mathcal{G}(\mathbf{r}\tau,\mathbf{r}\tau^+). \tag{20}$$

[1] In principle, we could still include another potential in H_0 and most of what we do in this problem still goes through when written in terms of exact eigenstates.

where τ^+ is infinitesimally later than τ. Next, define the Green function $\mathcal{G}_0(\mathbf{r}\tau, \mathbf{r}'\tau')$ in the absence of the potential $U(\mathbf{r})$ which satisfies the equation of motion

$$[\partial_\tau + H_0]\mathcal{G}(\mathbf{r}\tau, \mathbf{r}'\tau') = \delta(\mathbf{r} - \mathbf{r}')\delta(\tau - \tau'). \tag{21}$$

Multiply the equation of motion for $\mathcal{G}(\mathbf{r}\tau, \mathbf{r}'\tau')$ by $\mathcal{G}_0(\mathbf{r}\tau, \mathbf{r}'\tau')$ from the left (in the matrix sense, i.e., including integrations over space and time) and show that the equation of motion turns into the so-called Dyson equation

$$\mathcal{G}(\mathbf{r}\tau, \mathbf{r}'\tau') = \mathcal{G}_0(\mathbf{r}\tau, \mathbf{r}'\tau') - \int \mathrm{d}\mathbf{r}_1 \mathrm{d}\tau_1 \mathcal{G}_0(\mathbf{r}\tau, \mathbf{r}_1\tau_1) U(\mathbf{r}_1) \mathcal{G}(\mathbf{r}_1\tau_1, \mathbf{r}'\tau') \tag{22}$$

or

$$\mathcal{G} = \mathcal{G}_0 - \mathcal{G}_0 U \mathcal{G} \tag{23}$$

in matrix notation. Iterating this equation, we find an expansion in powers of U,

$$\mathcal{G} = \mathcal{G}_0 - \mathcal{G}_0 U \mathcal{G}_0 + \mathcal{G}_0 U \mathcal{G}_0 U \mathcal{G}_0 - \mathcal{G}_0 U \mathcal{G}_0 U \mathcal{G}_0 U \mathcal{G}_0 + \ldots \tag{24}$$

Thus, we find that to linear order in U, the density changes by

$$\delta n(\mathbf{r}, \tau) \simeq \mp \int \mathrm{d}\mathbf{r}_1 \mathrm{d}\tau_1 \mathcal{G}_0(\mathbf{r}\tau, \mathbf{r}_1\tau_1) U(\mathbf{r}_1) \mathcal{G}_0(\mathbf{r}_1\tau_1, \mathbf{r}\tau^+). \tag{25}$$

Consequently, we can write the polarization operator (albeit in imaginary time) as

$$\Pi_0(\mathbf{r}\tau, \mathbf{r}', \tau') = \pm \mathcal{G}_0(\mathbf{r}\tau, \mathbf{r}'\tau') \mathcal{G}_0(\mathbf{r}'\tau', \mathbf{r}\tau) \tag{26}$$

Write this in (Matsubara) frequency representation and perform the Matsubara sum (e.g., by writing the product of Green functions in terms of partial fractions and using the result of a previous problem). Finally, analytically continue the result, $i\omega_n \to \omega + i\eta$, to obtain the corresponding retarded correlation function and show that this reproduces the result of a previous problem set for the polarization operator.

Problem 3: Equation of motion approach to Hartree-Fock (10+10+5 points)

The Hartree-Fock approximation describes interacting systems in terms of an approximate non-interacting one. In this problem, we want to formulate the Hartree-Fock approximation in the framework of of the equation of motion for the single-particle Green function,

$$(\partial_\tau + H_0)\mathcal{G}(\mathbf{r}\tau, \mathbf{r}'\tau') + \int \mathrm{d}\mathbf{r}_1 \mathrm{d}\tau_1 v(\mathbf{r} - \mathbf{r}_1, \tau - \tau_1) \langle \mathrm{T}_\tau \psi(\mathbf{r}_1, \tau_1) \psi(\mathbf{r}, \tau) \psi^\dagger(\mathbf{r}_1, \tau_1^+) \psi^\dagger(\mathbf{r}', \tau') \rangle = \delta(\mathbf{r} - \mathbf{r}')\delta(\tau - \tau'). \tag{27}$$

Here, τ_1^+ is infinitesimally later than τ_1 and we consider a system with a Hamiltonian of the form

$$H = \int d\mathbf{r}\, \psi^\dagger(\mathbf{r}) \left(-\frac{\nabla^2}{2m} + U(\mathbf{r}) \right) \psi(\mathbf{r}) + \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') v(\mathbf{r} - \mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r}), \tag{28}$$

whose non-interacting part is denoted as H_0. We also defined $v(\mathbf{r} - \mathbf{r}_1, \tau - \tau_1) = v(\mathbf{r} - \mathbf{r}_1)\delta(\tau - \tau_1)$.

(a) To close the equation of motion, we have to approximate

$$\langle \mathrm{T}_\tau \psi(\mathbf{r}_1, \tau_1) \psi(\mathbf{r}, \tau) \psi^\dagger(\mathbf{r}_1, \tau_1^+) \psi^\dagger(\mathbf{r}', \tau') \rangle \tag{29}$$

in terms of the single-particle Green function $\mathcal{G}(\mathbf{r}\tau, \mathbf{r}'\tau')$. We can do that by neglecting the two-body interaction $v(\mathbf{r} - \mathbf{r}')$ in evaluating this correlator. Explain why this approximation yields

$$\langle \mathrm{T}_\tau \psi(\mathbf{r}_1, \tau_1) \psi(\mathbf{r}, \tau) \psi^\dagger(\mathbf{r}_1, \tau_1^+) \psi^\dagger(\mathbf{r}', \tau') \rangle \simeq \pm \mathcal{G}(\mathbf{r}\tau, \mathbf{r}'\tau') \mathcal{G}(\mathbf{r}_1\tau_1, \mathbf{r}_1\tau_1^+) + \mathcal{G}(\mathbf{r}\tau, \mathbf{r}_1\tau_1) \mathcal{G}(\mathbf{r}_1\tau_1, \mathbf{r}'\tau'). \tag{30}$$

(b) In the Hartree approximation, one keeps only the first of the two terms on the right hand side of the last equation. This yields the equation of motion

$$(\partial_\tau + H_0 + V_H)\mathcal{G}(\mathbf{r}\tau, \mathbf{r}'\tau') = \delta(\mathbf{r} - \mathbf{r}')\delta(\tau - \tau'), \tag{31}$$

where we defined the Hartree potential

$$V_H(\mathbf{r}) = \pm \int \mathrm{d}\mathbf{r}_1 v(\mathbf{r} - \mathbf{r}_1)\mathcal{G}(\mathbf{r}_1\tau, \mathbf{r}_1\tau^+). \tag{32}$$

Express the Hartree potential in terms of the eigenfunctions and eigenenergies of $H_0 + V_H$,

$$(H_0 + V_H)\phi_\alpha(\mathbf{r}) = \epsilon_\alpha\phi_\alpha(\mathbf{r}), \tag{33}$$

and find

$$V_H(\mathbf{r}) = \int \mathrm{d}\mathbf{r}_1 v(\mathbf{r} - \mathbf{r}_1) \sum_\alpha |\phi_\alpha(\mathbf{r}_1)|^2 n(\epsilon_\alpha). \tag{34}$$

Here, $n(\epsilon)$ denotes the Bose or Fermi function, respectively.

(c) Now consider also the second term in Eq. (30) which introduces the nonlocal Fock potential in addition,

$$(\partial_\tau + H_0 + V_H)\mathcal{G}(\mathbf{r}\tau, \mathbf{r}'\tau') \pm \int \mathrm{d}\mathbf{r}_1 V_F(\mathbf{r}, \mathbf{r}_1)\mathcal{G}(\mathbf{r}_1\tau, \mathbf{r}'\tau') = \delta(\mathbf{r} - \mathbf{r}')\delta(\tau - \tau'). \tag{35}$$

Also express the Fock potential in terms of the effective single-particle eigenfunctions and eigenenergies in Hartree-Fock approximation.

(d) **Bonus Problem** (You gain an additional 10 points and important insights): Consider the Hartree approximation and redo the derivation of the polarization operator. Note that the Hartree potential is a functional of the electron density. Show that this reproduces the RPA approximation discussed on an earlier problem set. If you are even more adventurous, you may want to try to understand the response function derived within the full Hartree-Fock approximation (or ask your tutor).