# Problem Set 6
# Quantum Field Theory and Many Body Physics (SoSe2018)

Due: Thursday, May 31, 2016 at the beginning of the lecture

In this problem set, we learn how to perform sums over Matsubara frequencies and study some aspects of Green functions and their equations of motion. The first problem is devoted to Matsubara sums which can be converted into contour integrals in the complex plane using the Bose or Fermi function. In the second 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 third 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.

**Problem 1: Matsubara sums** (5+5+5+5+5 points)

In evaluating the path integral for the harmonic chain, we encountered sums over bosonic Matsubara frequencies. They emerged because the fields we are integrating over are periodic in imaginary time with period $\hbar\beta$. It will turn out that this periodicity is a general feature of bosonic fields. In the class, we treated the two limiting cases of zero temperature (where the summation can be replaced by integration) and of $\hbar \to 0$ (where only one term of the sum survives). In this problem, we want to learn how to perform such sums in general by converting them into suitable contour integrals.

(a) Consider the Bose function

$$n_B(z) = \frac{1}{e^{\beta z} - 1} \tag{1}$$

in the complex plane, i.e., $z$ is a complex number. Show that it has poles for

$$z = i\hbar\Omega_n = \frac{2\pi i}{\beta} n \tag{2}$$

with $n$ an integer and $\Omega_n = (2\pi/\hbar\beta)n$. Show also that the residues of these poles are all equal to $1/\beta$.

(b) Now consider the important bosonic Matsubara sum

$$I = \frac{1}{\beta} \sum_{\Omega_n} \frac{e^{-i\Omega_n \tau}}{i\hbar\Omega_n - x} \tag{3}$$

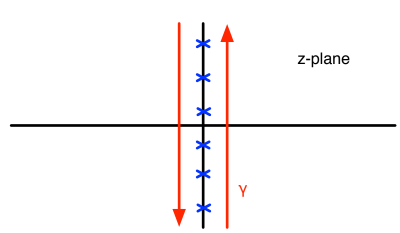
with $\tau \in [-\hbar\beta, \hbar\beta]$. Show that by Cauchy's theorem, this summation can be converted into the contour integral

$$I = \int_\gamma \frac{\mathrm{d}z}{2\pi i} \frac{e^{-z\tau/\hbar}}{z - x} \frac{-1}{e^{-\beta z} - 1} \tag{4}$$

for $\tau > 0$ and

$$I = \int_\gamma \frac{\mathrm{d}z}{2\pi i} \frac{e^{-z\tau/\hbar}}{z - x} \frac{1}{e^{\beta z} - 1} \tag{5}$$

for $\tau < 0$. In both cases, the contour $\gamma$ in the complex plane is given by



(c) Actually, so far both representations work independently of the sign of $\tau$. The sign of $\tau$ becomes important only in the next step in which we deform the contour. Show that for both integrals with the specified sign of $\tau$, the integrand vanishes exponentially for $|z| \to \infty$. (Remember that $|\tau| < \beta$.) Thus, we can add semicircles to the integration contour which go from $+i\infty$ to $-i\infty$ for Re$z > 0$ and from $-i\infty$ to $+i\infty$ for Re$z < 0$. These semicircles do not contribute to the integral. This yields two closed contours, one for Re$z < 0$ and another for Re$z > 0$. Use this to show that

$$I = -[n_B(x) + 1]e^{-x\tau/\hbar} \tag{6}$$

for $\tau > 0$ and

$$I = -n_B(x)e^{-x\tau/\hbar} \tag{7}$$

for $\tau < 0$.

(d) Now return to the harmonic chain. As shown in class, the equal-time correlation function

$$C(\mathbf{R}) = \langle[\phi(\mathbf{R}+\mathbf{r}) - \phi(\mathbf{r})]^2\rangle \tag{8}$$

can be computed from the path integral as

$$\mathbf{C}(\mathbf{R}) = \frac{1}{V}\sum_{\mathbf{q}} \frac{1}{\hbar\beta}\sum_{\Omega_n} \frac{\hbar \sin^2\left(\frac{\mathbf{q}\cdot\mathbf{R}}{2}\right)}{\rho\Omega_n^2 + \rho c^2 q^2} \tag{9}$$

where $\Omega_n = 2\pi n/(\hbar\beta)$ are the bosonic Matsubara frequencies. We had already evaluated the zero-temperature limit of the Matsubara sum in class. Now compute this correlation function for all temperatures (with the final result still written as a sum over momenta), performing the Matsubara sum with the technique that we just introduced. (In this case, the terms of the sum tend to 0 sufficiently fast that analogs of both integral expressions given above will work fine. Note that the sum in (b) above does not converge for $\tau = 0$.)

An alternative approach would be to note that

$$\sum_{\Omega_n} \frac{1}{\Omega_n^2 + c^2q^2} = \lim_{\eta\to 0^+}\sum_{\Omega_n} \frac{e^{i\Omega_n\eta}}{\Omega_n^2 + c^2q^2} = \lim_{\eta\to 0^+}\sum_{\Omega_n}\left[\frac{e^{i\Omega_n\eta}}{cq - i\Omega_n} + \frac{e^{i\Omega_n\eta}}{cq + i\Omega_n}\right]\frac{1}{2cq} \tag{10}$$

and then to use the result of (c) above. Here, we introduced a convergence factor $e^{i\Omega_n\eta}$ into the sum which is entirely inconsequential as long as we consider the original sum which converges nicely. But it is important once we decompose the original expression into its partial fractions. Now, the individual sums diverge logarithmically without convergence factor. This convergence factor is thus needed to separate the terms and sum them independently.

(e) Now consider a fermionic Matsubara sum. As we will see later in the course, fermionic fields $\psi(\tau)$ are antiperiodic in imaginary time, i.e.,

$$f(0) = -f(\hbar\beta). \tag{11}$$

Explain that such functions can be written as Fourier series

$$f(\tau) = \sum_{\epsilon_n} f(i\epsilon_n)e^{-i\epsilon_n\tau} \tag{12}$$

with fermionic Matsubara freqencies

$$\epsilon_n = \frac{\pi}{\hbar\beta}(2n+1). \tag{13}$$

Now follow the blueprint of the bosonic Matsubara sums (replacing the Bose by the Fermi function) to perform the fermionic sum

$$I = \frac{1}{\beta}\sum_{\epsilon_n} \frac{e^{-i\epsilon_n\tau}}{i\hbar\epsilon_n - x}. \tag{14}$$

**Problem 2: 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

$$\psi(\mathbf{r},t) = e^{iHt}\psi(\mathbf{r})e^{-iHt} \tag{15}$$

for a Hamiltonian of the form

$$H = \int d\mathbf{r}\, \psi^\dagger(\mathbf{r})\left(-\frac{\nabla^2}{2m} + U(\mathbf{r})\right)\psi(\mathbf{r}) + \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}')v(\mathbf{r}-\mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r}). \tag{16}$$

We will consider both bosons and fermions.

(a) Using the relation (prove!)

$$[A, BC] = [A, B]_\pm C \mp B[A, C]_\pm, \tag{17}$$

evaluate the commutator in the Heisenberg equation of motion

$$i\frac{\partial\psi}{\partial t} = [\psi, H] \tag{18}$$

to find

$$i\frac{\partial\psi(\mathbf{r},t)}{\partial t} = \left(-\frac{\nabla^2}{2m} + U(\mathbf{r})\right)\psi(\mathbf{r},t) + \int d\mathbf{r}'v(\mathbf{r}-\mathbf{r}')\psi^\dagger(\mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r}). \tag{19}$$

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

$$\left(-\frac{\nabla^2}{2m} + U(\mathbf{r})\right)\varphi_\alpha(\mathbf{r}) = \epsilon_\alpha\varphi_\alpha(\mathbf{r}). \tag{20}$$

To do so, expand

$$\psi(\mathbf{r},t) = \sum_\alpha \varphi_\alpha(\mathbf{r})c_\alpha(t) \tag{21}$$

and show that

$$c_\alpha(t) = e^{-i\epsilon_\alpha t}c_\alpha, \tag{22}$$

where $c_\alpha$ 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

$$\mathcal{G}(\mathbf{r}\tau,\mathbf{r}'\tau') = \langle \mathrm{T}_\tau\psi(\mathbf{r},\tau)\psi^\dagger(\mathbf{r}',\tau')\rangle, \tag{23}$$

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

$$\langle \mathrm{T}_\tau\psi(\mathbf{r}_1,\tau_1)\psi(\mathbf{r}_2,\tau_2)\psi^\dagger(\mathbf{r}_3,\tau_3)\psi^\dagger(\mathbf{r}_4,\tau_4)\rangle. \tag{24}$$

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 3: 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 $\Pi_0$ which we discussed in a previous problem set.

(a) Compute the finite temperature Green functions

$$
\begin{aligned}
G(\mathbf{r}t,\mathbf{r}'t') &= -i\langle \mathrm{T}\psi(\mathbf{r},t)\psi^\dagger(\mathbf{r}',t')\rangle, &(25)\\
G^R(\mathbf{r}t,\mathbf{r}'t') &= -i\,\theta(t-t')\langle[\psi(\mathbf{r},t),\psi^\dagger(\mathbf{r}',t')]_\mp\rangle, &(26)\\
G^A(\mathbf{r}t,\mathbf{r}'t') &= i\,\theta(t'-t)\langle[\psi(\mathbf{r},t),\psi^\dagger(\mathbf{r}',t')]_\mp\rangle, &(27)\\
\mathcal{G}(\mathbf{r}\tau,\mathbf{r}'\tau') &= \langle \mathrm{T}_\tau\psi(\mathbf{r},\tau)\psi^\dagger(\mathbf{r}',\tau')\rangle &(28)
\end{aligned}
$$

in the time domain.

(b) Fourier transform the result to obtain

$$
\begin{aligned}
G(\mathbf{r},r';\omega) &= \sum_\alpha \varphi_\alpha(\mathbf{r})\varphi^*_\alpha(\mathbf{r}')\left[\frac{1\pm n(\epsilon_\alpha)}{\omega-\epsilon_\alpha+i\eta}\mp\frac{n(\epsilon_\alpha)}{\omega-\epsilon_\alpha-i\eta}\right], &(29)\\
G^R(\mathbf{r},r';\omega) &= \sum_\alpha \frac{\varphi_\alpha(\mathbf{r})\varphi^*_\alpha(\mathbf{r}')}{\omega-\epsilon_\alpha+i\eta}, &(30)\\
G^A(\mathbf{r},r';\omega) &= \sum_\alpha \frac{\varphi_\alpha(\mathbf{r})\varphi^*_\alpha(\mathbf{r}')}{\omega-\epsilon_\alpha-i\eta}, &(31)\\
\mathcal{G}(\mathbf{r},r';i\omega_n) &= -\sum_\alpha \frac{\varphi_\alpha(\mathbf{r})\varphi^*_\alpha(\mathbf{r}')}{i\omega_n-\epsilon_\alpha}. &(32)
\end{aligned}
$$

Note that for many body systems, it is more appropriate to consider the thermal averages $\langle\dots\rangle$ 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 $\mu$.

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

$$[\partial_\tau + H_0 + U(\mathbf{r})]\mathcal{G}_0(\mathbf{r}\tau,\mathbf{r}'\tau') = \delta(\mathbf{r}-\mathbf{r}')\delta(\tau-\tau'), \tag{33}$$

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

$$n(\mathbf{r},\tau) = \pm\mathcal{G}(\mathbf{r}\tau,\mathbf{r}\tau^+). \tag{34}$$

where $\tau^+$ is infinitesimally later than $\tau$. 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

$$[\partial_\tau + H_0]\mathcal{G}_0(\mathbf{r}\tau,\mathbf{r}'\tau') = \delta(\mathbf{r}-\mathbf{r}')\delta(\tau-\tau'). \tag{35}$$

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

$$\mathcal{G}(\mathbf{r}\tau,\mathbf{r}'\tau') = \mathcal{G}_0(\mathbf{r}\tau,\mathbf{r}'\tau') - \int \mathrm{d}\mathbf{r}_1\mathrm{d}\tau_1\mathcal{G}_0(\mathbf{r}\tau,\mathbf{r}_1\tau_1)U(\mathbf{r}_1)\mathcal{G}(\mathbf{r}_1\tau_1,\mathbf{r}'\tau') \tag{36}$$

or

$$\mathcal{G} = \mathcal{G}_0 - \mathcal{G}_0 U\mathcal{G} \tag{37}$$

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

$$\mathcal{G} = \mathcal{G}_0 - \mathcal{G}_0U\mathcal{G}_0 + \mathcal{G}_0U\mathcal{G}_0U\mathcal{G}_0 - \mathcal{G}_0U\mathcal{G}_0U\mathcal{G}_0U\mathcal{G}_0 + \dots \tag{38}$$

[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.

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

$$\delta n(\mathbf{r},\tau) \simeq \mp \int \mathrm{d}\mathbf{r}_1 \mathrm{d}\tau_1 \mathcal{G}_0(\mathbf{r}\tau, \mathbf{r}_1\tau_1) U(\mathbf{r}_1) \mathcal{G}_0(\mathbf{r}_1\tau_1, \mathbf{r}\tau^+). \tag{39}$$

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

$$\Pi_0(\mathbf{r}\tau, \mathbf{r}', \tau') = \pm \mathcal{G}_0(\mathbf{r}\tau, \mathbf{r}'\tau') \mathcal{G}_0(\mathbf{r}'\tau', \mathbf{r}\tau) \tag{40}$$

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 the first 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.