Problem Set 5
Quantum Field Theory and Many Body Physics (SoSe2015)

Due: Monday, May 18, 2015 before the beginning of the class

In this problem set, we study various examples and aspects of linear response. We first consider a very simple linear response problem for the quantum harmonic oscillator. Then, we prove important general properties of response functions, including the Kramers-Kronig relations which are a direct consequence of causality and the associated analytic properties of the response function in the complex frequency plane. Finally, we consider the polarization operator, a very important response function in the theory of metals. We first compute it for free electrons and subsequently consider interacting electrons in the random-phase approximation.

Problem 1: Polarizability of a harmonic oscillator (5+5+5+5+5 points)

In this problem, we consider a very simple example for a response function, namely the polarizability χ of a charge e bound in a harmonic oscillator potential. The polarizability is defined through

$$d = \chi \mathcal{E}, \tag{1}$$

where d is the dipole moment, $d = ex$, and $\mathcal{E}$ the applied electric field. The Hamiltonian of the system is

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega_0^2 x^2 - ex\mathcal{E}. \tag{2}$$

(a) Use first order perturbation theory in a time-independent electric field $\mathcal{E}$ for the eigenstate $|\psi_n\rangle$ of H to derive the static polarizability χ. Specifically, according to first-order perturbation theory,

$$|\psi_n\rangle = |n\rangle + \sum_{m\neq n} |m\rangle \frac{\langle m| - e\mathcal{E}x|n\rangle}{E_n - E_m}, \tag{3}$$

where $|n\rangle$ denotes the eigenstates of the unperturbed harmonic oscillator ($\mathcal{E} = 0$) with eigenenergies $E_n = \hbar\omega_0(n + \frac{1}{2})$. Use this expression to compute the thermal expectation value

$$d = \sum_{n=0}^{\infty} \frac{e^{-\beta E_n}}{Z} \langle \psi_n | ex | \psi_n \rangle \tag{4}$$

to linear order in the applied field $\mathcal{E}$. (Here, the partition function is $Z = \sum_{n=0}^{\infty} e^{-\beta E_n}$.) You may find it useful that x couples only neighboring harmonic oscillator eigenstates with matrix elements (prove!)

$$\langle n+1|x|n\rangle = \frac{\ell_{\rm osc}}{\sqrt{2}} \sqrt{n+1} \tag{5}$$

$$\langle n-1|x|n\rangle = \frac{\ell_{\rm osc}}{\sqrt{2}} \sqrt{n} \tag{6}$$

in terms of the oscillator length $\ell_{\rm osc}^2 = \hbar/m\omega_0$. Eventually, you can perform the sum over n in the expression for d and find $\chi = \frac{e^2}{m\omega_0^2}$.

(b) Now define a dynamic polarizability as the response to a time-dependent electric field $\mathcal{E}(t)$ through

$$d(t) = \int_{\infty}^{\infty} dt' \, \chi(t, t') \mathcal{E}(t'). \tag{7}$$

Use the general Kubo formula derived in the class to obtain the Kubo formula

$$\chi(t,t') = \frac{ie^2}{\hbar}\theta(t-t')\langle[x(t),x(t')]\rangle \tag{8}$$

for the polarizability. Set up and solve the Heisenberg equation of motion for $x(t)$ (for the unperturbed harmonic oscillator!) to find

$$x(t) = x\cos\omega_0 t + \frac{p}{m\omega_0}\sin\omega_0 t. \tag{9}$$

Use this to evaluate the correlation function explicitly and find

$$\chi(t,t') = \frac{e^2}{m\omega_0}\theta(t-t')\sin(\omega_0(t-t')). \tag{10}$$

(c) Fourier transform $\chi(t,t')$ to the time domain and show that

$$\chi(\omega) = \frac{e^2/m}{\omega_0^2-(\omega+i\eta)^2}, \tag{11}$$

where η denotes a positive infinitesimal. Explain how this is related to the result in (a).

(d) Compute the thermal Green's function

$$\mathcal{G}(\tau,\tau') = \langle\mathcal{T}_\tau x(\tau)x(\tau')\rangle, \tag{12}$$

from the path integral for $E=0$, giving explicit results in the (Matsubara) frequency domain. Show that the retarded polarizability can be obtained from $\mathcal{G}(i\Omega)$ by analytical continuation.

(e) Compute the corresponding spectral function $\rho(\omega)$.

Problem 2: General properties of response functions (5+5+5+5+5 points)

In this problem we want to discuss some important general properties of response functions $D(t,t')$ in frequency representation. Consider a retarded Green's functions for bosonic operators, $\hat{A}$ and $\hat{B}$ with Lehmann representation

$$D(\omega) = \frac{1}{Z}\sum_{m,n}(e^{-\beta E_m}-e^{-\beta E_n})\frac{\langle m|\hat{A}|n\rangle\langle n|\hat{B}|m\rangle}{\omega-(E_n-E_m)+i\eta}, \tag{13}$$

and spectral representation

$$D(\omega) = \int\frac{d\omega}{2\pi}\frac{\rho(\omega')}{\omega-\omega'+i\eta} \tag{14}$$

in terms of the spectral function

$$\rho(\omega) = \frac{1}{Z}\sum_{n,m}(e^{-\beta E_m}-e^{-\beta E_n})\langle m|\hat{A}|n\rangle\langle n|\hat{B}|m\rangle\, 2\pi\delta(E_n-E_m-\omega). \tag{15}$$

(a) Use the Lehmann representation to show that

$$[D_{AB}(\omega)]^* = D_{A^\dagger B^\dagger}(-\omega) \tag{16}$$

Specifically, this implies for hermitian operators $\hat{A}$ and $\hat{B}$ that

$$\mathrm{Re}D(\omega) = \mathrm{Re}D(-\omega), \tag{17}$$

$$\mathrm{Im}\ \mathrm{D}(\omega) = -\mathrm{Im}D(-\omega), \tag{18}$$

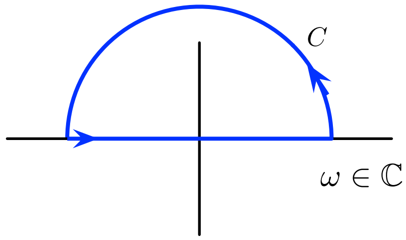

Figure 1: Integration contour

i.e., Re$D(\omega)$ is even in ω, Im D(ω) is odd.

(b) Show that the spectral function is real for the important case $\hat{B} = \hat{A}^\dagger$ (with $\hat{A}$ not necessarily a Hermitian operator).

(c) Prove the useful and frequently used identity (for infinitesimal η)

$$\frac{1}{x + i\eta} = \mathcal{P}(\frac{1}{x}) - i\pi\delta(x), \tag{19}$$

where $\mathcal{P}$ denotes the principal value and $\delta(x)$ is the Dirac δ-function. [Hint: The principal value can be represented as

$$\mathcal{P}\int dx\, \frac{f(x)}{x} = \lim_{\eta\to 0}\int dx\, f(x)\frac{x}{x^2+\eta^2}, \tag{20}$$

and

$$\frac{\eta}{x^2+\eta^2} = \pi\delta(x) \tag{21}$$

is a representation of the Dirac δ-dunction (why?).]

(d) Use the identity in (c) to show that for $\hat{B} = \hat{A}^\dagger$

$$\text{Im } D(\omega) = -\frac{1}{2}\rho(\omega), \tag{22}$$

and thus

$$D(\omega) = -\int \frac{d\omega'}{\pi}\frac{\text{Im}D(\omega)}{\omega - \omega' + i\eta}. \tag{23}$$

(e) Finally, we want to discuss a general relation between real and imaginary part of the response function $D(\omega)$ which is a direct consequence of causality, referred to as Kramer-Kronig relation. The Lehmann representation implies that $D(\omega)$ is an analytic function in the upper half of the complex ω-plane. Explain why

$$\int_C \frac{dz}{2\pi i}\frac{D(z)}{z - \omega + i\eta} = 0, \tag{24}$$

with the contour C specified in Fig. 1. Using that the integral over the semicircle vanishes when pushed to infinity, derive the Kramers-Kroning relation

$$D(\omega) = i\mathcal{P}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{D(\omega')}{\omega - \omega'}. \tag{25}$$

Specifically, this relation implies that

$$\text{Re}D(\omega) = -\mathcal{P}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\text{Im}D(\omega')}{\omega - \omega'}, \tag{26}$$

$$\text{Im}D(\omega) = \mathcal{P}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\text{Re}D(\omega')}{\omega - \omega'}. \tag{27}$$

Check that these relations work out for the response function in Eq. (11) above.

Problem 3: Polarization operator (10+5+10 points)

A very important response function describes the density response of a Fermi gas (e.g., non-interacting electrons) with chemical potential μ to an applied electric potential $\phi(\mathbf{r}, t)$,

$$\delta\rho(\boldsymbol{r}, t) = -e^2 \int d\mathbf{r}' dt'\, \Pi_0(\mathbf{r}t, \mathbf{r}'t')\phi(r', t'). \tag{28}$$

Since the system is translationally invariant in both space and time, we have

$$\delta\rho(\mathbf{q}, \omega) = -e^2 \Pi_0(\mathbf{q}, \omega)\phi(\mathbf{q}, \omega). \tag{29}$$

Π_0 is often referred to as the polarization operator. It can be computed by applying the Lehmann representation to a single electron system with occupation probability

$$n_k = \frac{1}{e^{\beta(\epsilon_k - \mu)} + 1} \tag{30}$$

of the momentum states $|k\rangle$. The charge density is

$$\hat{\rho}(\mathbf{r}) = e\delta(\mathbf{r} - \hat{\mathbf{r}}), \tag{31}$$

and the electric potential couples to the electron through

$$H_{int} = e\phi(\hat{\mathbf{r}}) = \int d\mathbf{r}\, \hat{\rho}(\mathbf{r})\phi(\mathbf{r}). \tag{32}$$

Correspondingly, we obtain in Fourier representation $\hat{\rho}(\mathbf{q}) = e^{-i\mathbf{q}\cdot\hat{\mathbf{r}}}$ and $H_{int} = \frac{1}{V}\sum_q \hat{\rho}(-\mathbf{q})\phi(\mathbf{q})$. Using this in the Lehmann representation for the Kubo formula for Π_0, we find (with $\epsilon_k = \mathbf{k}^2/2m$)

$$\Pi_0(\mathbf{q}, \omega) = -\frac{1}{e^2}\frac{1}{V}\sum_{\mathbf{k}\mathbf{k}'}(n_{\mathbf{k}} - n_{\mathbf{k}'})\frac{\langle\mathbf{k}|\hat{\rho}(\mathbf{q})|\mathbf{k}'\rangle\langle\mathbf{k}'|\hat{\rho}(-\mathbf{q})|\mathbf{k}\rangle}{\omega + \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'} + i\eta}. \tag{33}$$

Please make sure that you understand the logic leading to this expression.

(a) Evaluate the matrix elements $\langle\mathbf{k}|\hat{\rho}(\mathbf{q})|\mathbf{k}'\rangle$ and show that

$$\Pi_0(\mathbf{q}, \omega) = -\frac{1}{V}\sum_{\mathbf{k}}\frac{n_{\mathbf{k}} - n_{\mathbf{k}+\mathbf{q}}}{\omega + \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'+\mathbf{q}} + i\eta} \tag{34}$$

(b) Evaluate both $\mathrm{Re}\Pi_0(\mathbf{q}, \omega)$ and $\mathrm{Im}\Pi_0(\mathbf{q}, \omega)$ explicitly in 3d by performing the integration over $\mathbf{k}$ ($\frac{1}{V}\sum_{\mathbf{k}} \to \int \frac{d^3\mathbf{k}}{(2\pi)^3}$). [Hint: See, e.g. the book by Fetter and Walecka, p158ff, if you need help.]

(c) Imagine now a Fermi system of charged particles, e.g. electrons. Let us also assume that the average electronic charge density is compensated by a uniform and rigid background of opposite charge (representing the ion cores in a solid). Then, the change in the electronic charge density $\delta\rho(\mathbf{r}t)$ is itself producing an induced electric potential, $\phi_{\mathrm{ind}}(\mathbf{r}, t)$,

$$\phi_{\mathrm{ind}}(\mathbf{r}, t) = \int d\mathbf{r}'\, \frac{\delta\rho(\mathbf{r}', t)}{|\mathbf{r} - \mathbf{r}'|}. \tag{35}$$

The actual induced charge density is thus a response to the total potential

$$\phi_{\mathrm{tot}}(\mathbf{r}, t) = \phi(\mathbf{r}, t) + \phi_{\mathrm{ind}}(\mathbf{r}, t), \tag{36}$$

which is the sum of the external potential $\phi(\mathbf{r},t)$ and the induced potential. Thus,

$$\delta\rho(\mathbf{q},\omega) = -e^2 \int d\mathbf{r}'dt'\, \Pi_0(\mathbf{r}t,\mathbf{r}'t') \left(\phi(\mathbf{r}',t') + \phi_{\text{ind}}(\mathbf{r}',t')\right). \tag{37}$$

Note that this is an approximation (called RPA or random phase approximation for historical reasons) in that we neglect the effects of the Coulomb interaction on Π_0. Show that this equation can be Fourier transformed to give

$$\delta\rho(\mathbf{q},\omega) = -e^2\Pi_0(\mathbf{q},\omega)\left(\phi(\mathbf{q},\omega) + \phi_{\text{ind}}(\mathbf{q},\omega)\right). \tag{38}$$

Moreover, show that

$$\phi_{ind}(\mathbf{q},\omega) = \frac{1}{e^2}v(\mathbf{q})\delta\rho(\mathbf{q},\omega), \tag{39}$$

with $v(\mathbf{q}) = \frac{4\pi e^2}{\mathbf{q}^2}$. Defining a response function $\Pi(\mathbf{q},\omega)$ describing the density response of the interacting Fermi system to the externally applied potential $\phi(\mathbf{q},\omega)$, i.e.,

$$\delta\rho(\mathbf{q},\omega) = -e^2\Pi(\mathbf{q},\omega)\phi(\mathbf{q},\omega), \tag{40}$$

show that

$$\Pi(\mathbf{q},\omega) = \frac{\Pi_0(\mathbf{q},\omega)}{1 + v(\mathbf{q})\Pi_0(\mathbf{q},\omega)}. \tag{41}$$

Use this to find

$$\phi_{\text{tot}}(\mathbf{q},\omega) = \frac{1}{1 + v(\mathbf{q})\Pi_0(\mathbf{q},\omega)}\phi(\mathbf{q},\omega). \tag{42}$$

Compute the total potential in real space within the Thomas-Fermi approximation ($\Pi_0(\mathbf{q},\omega) = \nu_0$, where ν_0 is the density of states at the Fermi energy) for a point charge e inserted into the system, i.e., for

$$\phi(\mathbf{q},\omega) = \frac{4\pi e}{\mathbf{q}^2}. \tag{43}$$

Explain your result in physical terms (screening).