

Problem Set 5

Quantum Field Theory and Many Body Physics (SoSe2018)

Due: Thursday, May 24, 2018 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

$$d = \chi \mathcal{E}, \quad (1)$$

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

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

(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,

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

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

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

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!)

$$\langle n+1 | x | n \rangle = \frac{\ell_{\text{osc}}}{\sqrt{2}} \sqrt{n+1} \quad (5)$$

$$\langle n-1 | x | n \rangle = \frac{\ell_{\text{osc}}}{\sqrt{2}} \sqrt{n} \quad (6)$$

in terms of the oscillator length $\ell_{\text{osc}}^2 = \hbar/m\omega_0$. 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

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

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

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

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

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

Use this to evaluate the correlation function explicitly and find

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

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

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

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

(d) Compute the thermal Green's function

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

from the path integral for $\mathcal{E} = 0$, 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

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

and spectral representation

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

in terms of the spectral function

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

(a) Use the Lehmann representation to show that

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

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

$$\text{Re} D(\omega) = \text{Re} D(-\omega), \quad (17)$$

$$\text{Im} D(\omega) = -\text{Im} D(-\omega), \quad (18)$$

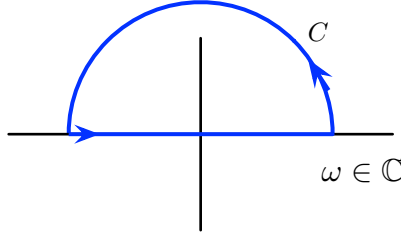


Figure 1: Integration contour

i.e., $\text{Re}D(\omega)$ is even in ω , $\text{Im} D(\omega)$ 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 $\eta > 0$)

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

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

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

and

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

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

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

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

and thus

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

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

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

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

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

Specifically, this relation implies that

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

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

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 $\phi(\mathbf{r}, t)$,

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

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

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

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

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

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

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

and the electric potential couples to the electrons through

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

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

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

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

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

(b) Evaluate both $\text{Re}\Pi_0(\mathbf{q}, \omega)$ and $\text{Im}\Pi_0(\mathbf{q}, \omega)$ explicitly in 3d by performing the integration over \mathbf{k} ($\frac{1}{V} \sum_{\mathbf{k}} \rightarrow \int \frac{d^3\mathbf{k}}{(2\pi)^3}$). [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, $\phi_{ind}(\mathbf{r}, t)$,

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

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

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

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

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

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

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

Moreover, show that

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

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.,

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

show that

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

Use this to find

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

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

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

Explain your result in physical terms (screening).