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Quantum Many-Body Systems

3. Exercise Sheet

10 Lindhardt function in the long-time and long-wavelength limit

(a) Consider the expression we obtained for the dynamic structure factor of a free electron gas, i.e., equation (9.2)

$$S(\boldsymbol{q},\omega) = \frac{1}{\hbar V}\sum_{\boldsymbol{k},\sigma} n_{\boldsymbol{k},\sigma}(1-n_{\boldsymbol{k}+\boldsymbol{q},\sigma})\delta(\omega-\xi_{\boldsymbol{k},\boldsymbol{q}}) \tag{10.1}$$

Show that you can rewrite this equation as

$$S(\boldsymbol{q},\omega) = \frac{1}{\hbar V(1-e^{-\beta\hbar\omega})}\sum_{\boldsymbol{k},\sigma} (n_{\boldsymbol{k},\sigma}-n_{\boldsymbol{k}+\boldsymbol{q},\sigma})\delta(\omega-\xi_{\boldsymbol{k},\boldsymbol{q}}) \tag{10.2}$$

with $\xi_{\boldsymbol{k},\boldsymbol{q}} = \frac{1}{\hbar}(\varepsilon_{\boldsymbol{k}+\boldsymbol{q}}-\varepsilon_{\boldsymbol{k}})$ where $\varepsilon_{\boldsymbol{k}} = \dfrac{\hbar^2k^2}{2m}$.

(1 point)

Hint: Use the identity $n_{\boldsymbol{k},\sigma}(1-n_{\boldsymbol{k}+\boldsymbol{q},\sigma}) = \dfrac{n_{\boldsymbol{k},\sigma}-n_{\boldsymbol{k}+\boldsymbol{q},\sigma}}{1-e^{-\beta\xi_{\boldsymbol{k},\boldsymbol{q}}}}$ in (10.1).

(b) Substitute (10.2) in (3.6) (see problem sheet 1) and perform the integral over ω' to obtain

$$\chi(\boldsymbol{q},\omega) = -\frac{1}{\hbar V}\sum_{\boldsymbol{k},\sigma}\frac{n_{\boldsymbol{k},\sigma}-n_{\boldsymbol{k}+\boldsymbol{q},\sigma}}{\omega+i\delta-\xi_{\boldsymbol{k},\boldsymbol{q}}}. \tag{10.3}$$

This is an alternative representation of $\chi(\boldsymbol{q}, \omega)$ that is more useful for the solution of this problem.
(2 points)

(c) Show that in the limit $\boldsymbol{q} \to 0$ and to linear order, one has $\xi_{\boldsymbol{k},\boldsymbol{q}} \approx \dfrac{\hbar \boldsymbol{k} \cdot \boldsymbol{q}}{m}$ and $n_{\boldsymbol{k},\sigma} - n_{\boldsymbol{k}+\boldsymbol{q},\sigma} \approx \dfrac{\partial n_{\boldsymbol{k},\sigma}}{\partial \mu} \cdot \dfrac{\hbar^2 \boldsymbol{k} \cdot \boldsymbol{q}}{m}$. Note that $n_{\boldsymbol{k},\sigma} = \dfrac{1}{e^{\beta(\varepsilon_{\boldsymbol{k}})} + 1}$.
(2 points)

(d) Hence, show that in such a limit

$$\chi(\boldsymbol{q}, \omega) = -\frac{1}{V} \sum_{\boldsymbol{k},\sigma} \frac{\boldsymbol{q} \cdot \boldsymbol{v}_{\boldsymbol{k}}}{\omega + i\delta - \boldsymbol{q} \cdot \boldsymbol{v}_{\boldsymbol{k}}} \cdot \frac{\partial n_{\boldsymbol{k},\sigma}}{\partial \mu}, \tag{10.4}$$

where $\boldsymbol{v}_{\boldsymbol{k}} = \dfrac{\hbar \boldsymbol{k}}{m}$ is the velocity of a particle with wave-number $\boldsymbol{k}$.
(2 points)

(e) Show from (10.4) that $\lim_{\boldsymbol{q} \to 0} \chi(\boldsymbol{q}, 0) = n^2 \kappa_T$ and hence that the response function $\chi(\boldsymbol{q}, \omega)$ satisfies the compressibility sum rule.
(2 points)

(f) At $T = 0$, $\dfrac{\partial n_{\boldsymbol{k},\sigma}}{\partial \mu} = \delta(\varepsilon_{\boldsymbol{k}} - \mu)$. Thus, show that

$$\chi(\boldsymbol{q}, 0) = \frac{1}{V} \sum_{\boldsymbol{k},\sigma} \delta(\varepsilon_{\boldsymbol{k}} - \mu) = \frac{m k_F}{\pi^2 \hbar^2}. \tag{10.5}$$

The quantity $\rho(\mu) = \dfrac{1}{V} \sum_{\boldsymbol{k},\sigma} \delta(\varepsilon_{\boldsymbol{k}} - \mu) = \dfrac{m k_F}{\pi^2 \hbar^2}$ is the density of states (per unit volume) at the Fermi level.
(2 points)
Hint: In the limit of large V, convert the sum above in an integral over $\boldsymbol{k}$ (see exercise sheet 2) and perform such an integral.

(g) Use (10.5) to show that $\kappa_{T=0} = \dfrac{3^{1/3} m}{\hbar^2 \pi^{4/3} n^{5/3}}$.
(2 points)
Hint: Note that $k_F = (3\pi^2 n)^{1/3}$.

(h) Consider a classical perfect gas, with the equation of state $P = n k_B T$. Show that $\kappa_T = -\dfrac{1}{V} \dfrac{\partial V}{\partial P}\Big|_{T,N} = \dfrac{1}{P} = \dfrac{1}{n k_B T}$.
(2 points)

(i) In the limit $T \to 0$, the compressibility of a classical perfect gas would diverge (this result is meaningless, as the classical perfect gas model is only valid at sufficiently

high temperatures and low densities). However, the compressibility of the free Femi gas does not diverge at zero temperature and, moreover, it decreases with a higher power of the density (i.e. with $n^{-5/3}$). Remember that in a free Fermi gas, there are no interactions between the fermions. Thus, what physical effect is responsible for keeping the compressibility finite at $T = 0$?
(2 points)

(j) Show from (10.4) that at $T = 0$ (for $\boldsymbol{q} \neq 0$), one obtains

$$\chi(\boldsymbol{q}, \omega) = \rho(\mu)\Big[1 - \frac{\lambda}{2} \ln\Big(\frac{\lambda + 1}{\lambda - 1}\Big)\Big], \tag{10.6}$$

where $\lambda = \dfrac{\omega}{q v_F}$, with $v_F = \dfrac{\hbar k_F}{m}$ being the velocity of a particle at the Fermi surface. The quantity $\rho(\mu)$ is the density of states at the Fermi level, introduced above.
(4 extra points)
Hint: Use $\dfrac{\partial n_{\boldsymbol{k},\sigma}}{\partial \mu} = \delta(\varepsilon_{\boldsymbol{k}} - \mu)$ in (10.4), convert the sum over $\boldsymbol{k}$ into an integral and perform such integral using spherical coordinates. Do note that since $\boldsymbol{q}$ is a fixed vector, you can choose the z-axis in the integral over $\boldsymbol{k}$ to be along $\boldsymbol{q}$.

11 Analytic properties of the causal Green function

The properties of the retarded, advanced, and Matsubara Green functions were covered extensively during class. Here, we will consider instead the properties of the causal Green function in real time. This quantity is defined, in a given basis of operators, by

$$G_{\alpha\gamma}(t, t') = -\frac{i}{\hbar}\langle T\{\hat{c}_\alpha(t)\hat{c}^\dagger_\gamma(t')\}\rangle \tag{11.1}$$

$$= -\frac{i}{\hbar}\big[G^>_{\alpha\gamma}(t, t')\Theta(t - t') + \zeta G^<_{\alpha\gamma}(t, t')\Theta(t' - t)\big], \tag{11.2}$$

where $\zeta = +1$ ($\zeta = -1$) for bosons (fermions), T is the time-ordering operator and $G^>_{\alpha\gamma}(t, t') = \langle \hat{c}_\alpha(t)\hat{c}^\dagger_\gamma(t')\rangle$, $G^<_{\alpha\gamma}(t, t') = \langle \hat{c}^\dagger_\alpha(t')\hat{c}_\gamma(t)\rangle$.

(a) The above functions can be written as

$$G^>_{\alpha\gamma}(t, t') = \frac{1}{Z_0}\mathrm{Tr}\Big(\hat{c}_\alpha(t)\hat{c}^\dagger_\gamma(t')e^{-\beta(\hat{H}_0 - \mu\hat{N})}\Big), \tag{11.3}$$

and

$$G^<_{\alpha\gamma}(t, t') = \frac{1}{Z_0}\mathrm{Tr}\Big(\hat{c}^\dagger_\gamma(t')\hat{c}_\alpha(t)e^{-\beta(\hat{H}_0 - \mu\hat{N})}\Big), \tag{11.4}$$

where $\hat{H}_0$ is a many-body Hamiltonian such that $[\hat{N}, \hat{H}_0] = 0$, and $\hat{c}_\alpha(t) = e^{i\hat{H}_0 t/\hbar}\hat{c}_\alpha e^{-i\hat{H}_0 t/\hbar}$ and $\hat{c}^\dagger_\gamma(t') = e^{i\hat{H}_0 t/\hbar}\hat{c}^\dagger_\gamma e^{-i\hat{H}_0 t/\hbar}$ are the annihilation and creation operators in the Heisenberg representation. Show from their representation that they only depend on the difference $t - t'$.
(2 points)

(b) Thus, it is enough to consider $G^{>}_{\alpha\gamma}(t) = \langle \hat{c}_\alpha(t)\hat{c}^\dagger_\gamma\rangle$ and $G^{<}_{\alpha\gamma}(t) = \langle \hat{c}^\dagger_\gamma \hat{c}_\alpha(t)\rangle$. Show that these functions are connected by the identity $G^{>}_{\alpha\gamma}(t - i\beta\hbar) = e^{-\beta\mu} G^{<}_{\alpha\gamma}(t)$.
(3 points)
Hint: Use the identity $e^{-\beta\mu\hat{N}}\hat{c}^\dagger_\gamma e^{\beta\mu\hat{N}} = \hat{c}^\dagger_\gamma e^{-\beta\mu}$ (proving it is part of the exercise) in the expression for $G^{>}_{\alpha\gamma}(t - i\beta\hbar)$ and then apply the cyclic invariance of the trace.

(c) Use the result proven in (b) to show that the Fourier transforms of these functions, $G^{>}_{\alpha\gamma}(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} G^{>}_{\alpha\gamma}(t)$, and are related by $G^{<}_{\alpha\gamma}(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} G^{<}_{\alpha\gamma}(t)$ are related by

$$G^{<}_{\alpha\gamma}(\omega) = e^{-\beta(\hbar\omega - \mu)} G^{>}_{\alpha\gamma}(\omega). \tag{11.5}$$

(2 points)
Hint: Substitute $G^{<}_{\alpha\gamma}(t) = e^{\beta\mu} G^{>}_{\alpha\gamma}(t - i\beta\hbar)$ in its Fourier transform and express $G^{>}_{\alpha\gamma}(t - i\beta\hbar)$ in terms of $G^{>}_{\alpha\gamma}(\omega)$ itself.

(d) Since $G^{>}_{\alpha\gamma}(t - t')$ and $G^{<}_{\alpha\gamma}(t - t')$ only depend on the difference $t - t'$, the same is true for $G_{\alpha\gamma}(t, t')$, see (11.1). Thus, one can also consider the Fourier transform $G_{\alpha\gamma}(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} G_{\alpha\gamma}(t)$. Show that $G_{\alpha\gamma}(\omega)$ is related to $G^{>}_{\alpha\gamma}(\omega)$ by

$$G_{\alpha\gamma}(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi\hbar} G^{>}_{\alpha\gamma}(\omega')\Big(\frac{1}{\omega - \omega' + i\delta} - \frac{\zeta e^{-\beta(\hbar\omega' - \mu)}}{\omega - \omega' - i\delta}\Big), \tag{11.6}$$

where the infinitesimal factors $\pm i\delta$ are introduced in the Fourier exponents to ensure convergence.
(3 points)

(e) Define the function $A_{\alpha\gamma}(\omega) = G^{>}_{\alpha\gamma}(\omega)(1 - \zeta e^{-\beta(\hbar\omega - \mu)})/(2\pi)$ (spectral density). Show that one can write (11.6) as

$$G_{\alpha\gamma}(\omega) = P\int_{-\infty}^{\infty} \frac{d\omega'}{\hbar}\frac{A_{\alpha\gamma}(\omega')}{\omega - \omega'} - \frac{i\pi}{\hbar} A_{\alpha\gamma}(\omega) \begin{cases} \tanh^{-1}\big(\dfrac{\beta(\hbar\omega - \mu)}{2}\big) \\ \tanh\big(\dfrac{\beta(\hbar\omega - \mu)}{2}\big) \end{cases}, \tag{11.7}$$

where the result in the top of the brackets applies in the case of bosons and the result in the bottom applies in the case of fermions. The symbol P denotes the principal part of the integral.
(2 points) Hint: Use the Dirac relation $\dfrac{1}{\omega - \omega' \pm i\delta} = P\dfrac{1}{\omega - \omega'} \mp i\pi\delta(\omega - \omega')$ in (11.6).

(f) Show that $G^{>}_{\alpha\gamma}(\omega)$ has the following Lehmann representation in terms of the eigenstates $|m\rangle$ and $|n\rangle$ of $\hat{H}_0$

$$G^{>}_{\alpha\gamma}(\omega) = \frac{2\pi}{Z_0}\sum_{m,n}\langle m|\hat{c}_\alpha|n\rangle\langle n|\hat{c}^\dagger_\gamma|m\rangle \delta(\omega - \omega_{nm}) e^{-\beta(E_M - \mu N_m)}, \tag{11.8}$$

where $\omega_{nm} = \frac{1}{\hbar}(E_n - E_m)$.
(2 points)
Hint: First obtain the Lehmann representation for $G^<_{\alpha\gamma}(t)$ and then Fourier transform the result obtained.

(g) Show from (11.8) that $G^>_{\alpha\alpha}(\omega)$ is a real (and positive definite) function. Hence show that $A_{\alpha\alpha}(\omega)$ is also real, and being positive definite for fermions and being positive or negative in the case of bosons, depending on whether $\hbar\omega > \mu$ or $\hbar\omega < \mu$.
(2 points)

(h) Show that $G_{\alpha\alpha}(\omega)$ obeys the following Kramers-Kronig relation

$$\mathrm{Re}G_{\alpha\alpha}(\omega) = -P\int_{-\infty}^{\infty} \frac{d\omega'}{\pi}\frac{\mathrm{Im}G_{\alpha\alpha}(\omega)}{\omega - \omega'}\begin{cases}\tanh\left(\frac{\beta(\hbar\omega-\mu)}{2}\right)\\ \tanh^{-1}\left(\frac{\beta(\hbar\omega-\mu)}{2}\right)\end{cases} \tag{11.9}$$

where the result in the top of the bracket appliesto bosons and the result in the bottom in the case of fermions.
(2 points)

(i) Show that $A_{\alpha\gamma}(\omega)$ is given by the following Lehmann representation

$$A_{\alpha\gamma}(\omega) = \frac{1}{Z_0}\sum_{m,n}\langle m|\hat{c}_\alpha|n\rangle\langle n|\hat{c}^\dagger_\gamma|m\rangle\delta(\omega - \omega_{nm})\left(e^{-\beta(E_m-\mu N_m)} - \zeta e^{-\beta(E_n-\mu N_n)}\right), \tag{11.10}$$

where $N_n = N_m + 1$. Show from (11.10) that $\int_{-\infty}^{\infty} d\omega\, A_{\alpha\gamma}(\omega) = \delta_{\alpha,\gamma}$.
(4 extra points)

(j) Suppose that $\hat{H}_0 = \sum_\nu \varepsilon_\nu \hat{c}^\dagger_\nu \hat{c}_\nu$, i.e., $\hat{H}_0$ is a one-body Hamiltonian and we consider the Green function in the basis that diagonalizes $\hat{H}_0$. Show that

(i) $G^>_{\alpha\gamma}(\omega) = 2\pi\delta_{\alpha,\gamma}(1+\zeta n_\alpha)\delta(\omega - \omega_\alpha)$, where $n_\alpha = \frac{1}{e^{\beta(\varepsilon_\alpha-\mu)} - \zeta}$ and $\omega_\alpha = \varepsilon/\hbar$.
(2 points)
Hint: Use the results of problem 6a and 6b (see exercise sheet 2) to compute $G^>_{\alpha\gamma}(t)$ and then perform a Fourier transform.

(ii) Show that $A_{\alpha\gamma}(\omega) = \delta_{\alpha,\gamma}\delta(\omega - \omega_\alpha)$ and show that these functions obey the sum rule derived above, $\int_{-\infty}^{\infty} d\omega\, A_{\alpha\gamma}(\omega) = \delta_{\alpha,\gamma}$.
(2 points)

(iii) Finally, show that $G_{\alpha\gamma}(\omega)$ is given in this case by

$$G_{\alpha\gamma}(\omega) = \frac{\delta_{\alpha,\gamma}}{\hbar}\left(P\frac{1}{\omega - \omega_\alpha} - i\pi\delta(\omega - \omega_\alpha)\begin{cases}\tanh^{-1}\left(\frac{\beta(\hbar\omega-\mu)}{2}\right)\\ \tanh\left(\frac{\beta(\hbar\omega-\mu)}{2}\right)\end{cases}\right), \tag{11.11}$$

where again the result in the top of the bracket applies in the case of bosons and the result in the bottom in the case of fermions.
(1 point)

12 Matsubara sums

Consider the function $f(\omega) = \sum_{n=-\infty}^{\infty} \frac{1}{(2n\pi)^2 + \omega^2}$,defined for any $\omega \neq 0$. This function is positive definite. The goal of this exercise is to compute this quantity and similar ones which later will prove useful when one performs summations over Matsubara frequencies.

(a) Show that one can express $f(\omega) = \oint_C \frac{dz}{2\pi i} \frac{1}{e^z - 1} \frac{1}{\omega^2 - z^2}$, where the contour is the union of the circles that surround each pole of $\frac{1}{e^z - 1}$, see figure 1.
(2 points)

(b) Show that by deforming C over two infinite semi-circles to the right and left of the imaginary axis (see figure 1) and by using the residue theorem, one has $f(\omega) = \frac{1}{2\omega} \tanh^{-1} \left(\frac{\omega}{2}\right)$.
(2 points)

(c) Consider $g(\omega) = \sum_{n=-\infty}^{\infty} \frac{1}{(n\pi)^2 + \omega^2}$. By appropriately expressing it in terms of $f(\omega)$, show that one has $g(\omega) = \frac{1}{\omega} \tanh^{-1} \left(\omega\right)$.
(1 point)

(d) Finally, consider $h(\omega) = \sum_{n=-\infty}^{\infty} \frac{1}{((2n+1)\pi)^2 + \omega^2}$. One could also express this sum as a contour integral, but there is a simpler way to compute it. First, show that $h(\omega) = g(\omega) - f(\omega)$. Then, show from the results above that $h(\omega) = \frac{1}{2\omega} \tanh \left(\frac{\omega}{2}\right)$.
(3 points)

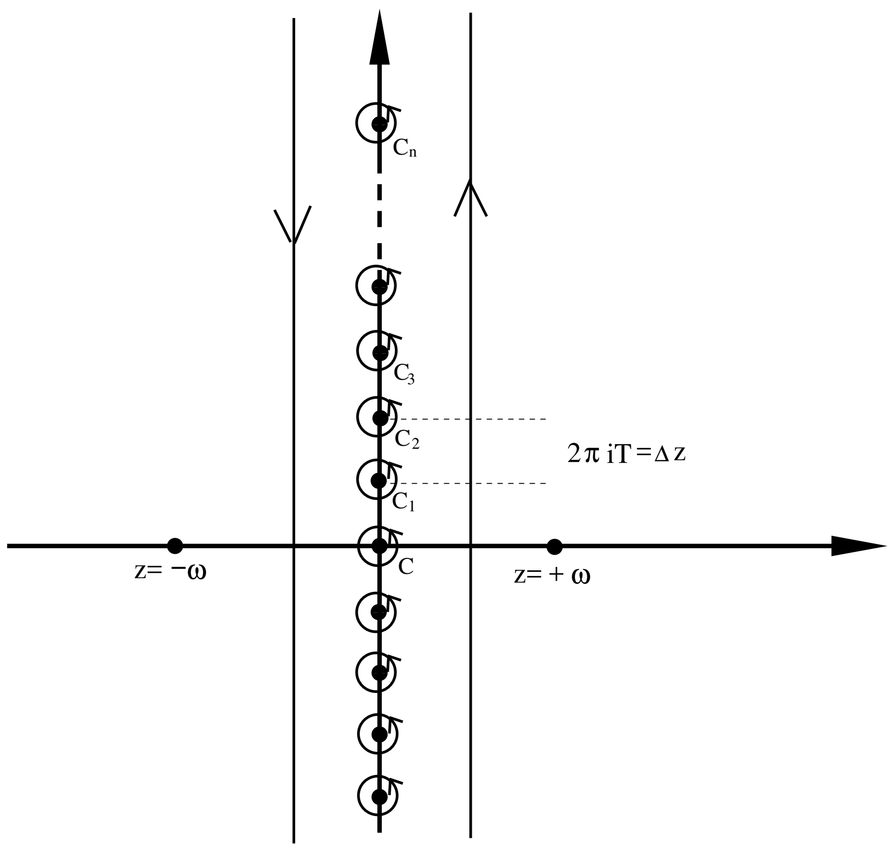

Figure 12.1: Contour used to express summation as a contour integral.