Group study: Linear response theory

Project 2: Correlation energy

Let's consider an interacting electron gas in 3D which provides a first approximation to a metal or a plasma. We will calculate corrections to the ground-state energy due to the Coulomb interaction:

$$\hat{U} = \frac{1}{2V} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{q},\sigma_1,\sigma_2} u(\boldsymbol{q}) \hat{a}^\dagger_{\boldsymbol{k}_1+\boldsymbol{q},\sigma_1} \hat{a}^\dagger_{\boldsymbol{k}_2-\boldsymbol{q},\sigma_2} \hat{a}_{\boldsymbol{k}_2,\sigma_2} \hat{a}_{\boldsymbol{k}_1,\sigma_1}$$

where $u(\boldsymbol{q}) = \frac{4\pi e^2}{|\boldsymbol{q}|^2}$ in 3D and σ_1, σ_2 represent the spin index.

1. (20 pts) **Exchange energy of 3D electron gas**

   The exchange contribution to the Coulomb interaction, which arises from the anti-symmetry of the wave functions, is given by

   $$\hat{U}^{(\mathrm{ex})} = \sum_{\boldsymbol{k},\sigma} \varepsilon^{(\mathrm{ex})}_{\boldsymbol{k}} \hat{a}^\dagger_{\boldsymbol{k},\sigma} \hat{a}_{\boldsymbol{k},\sigma} - \left\langle \hat{U}^{(\mathrm{ex})} \right\rangle,$$

   where

   $$\varepsilon^{(\mathrm{ex})}_{\boldsymbol{k}} = -\frac{1}{V} \sum_{\boldsymbol{k}'} u(\boldsymbol{k}-\boldsymbol{k}') n_{\boldsymbol{k}',\sigma}.$$

   (a) Show that at $T = 0$,

   $$\varepsilon^{(\mathrm{ex})}_{\boldsymbol{k}} = -\frac{2e^2 k_{\mathrm{F}}}{\pi} F\left(\frac{k}{k_{\mathrm{F}}}\right),$$

   where $F(z)$ is defined by

   $$F(z) = \int_{|\boldsymbol{z}'|<1} \frac{d^3 z'}{4\pi} \frac{1}{|\boldsymbol{z}-\boldsymbol{z}'|^2}.$$

   (b) Show that $F(z)$ is given by

   $$F(z) = \frac{1}{2} - \frac{z^2-1}{4z} \ln\left|\frac{z+1}{z-1}\right|.$$

   For convenience, locate $\boldsymbol{z}$ along the z-axis and integrate with $\boldsymbol{z}'$ using the spherical coordinates.

   $*$ This is the Lindhard function which also appeared in Problem 2 of Project 1.

   (c) The exchange energy $E_{\mathrm{ex}} = \left\langle \hat{U}^{(\mathrm{ex})} \right\rangle$ is then given by

   $$E_{\mathrm{ex}} = \frac{V}{2} \int \frac{d^3 k}{(2\pi)^3} \sum_{\sigma} \varepsilon^{(\mathrm{ex})}_{\boldsymbol{k}} n_{\boldsymbol{k},\sigma}.$$

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Show that the exchange energy per particle is given by

$$\varepsilon_{\rm ex} = \frac{E_{\rm ex}}{N} = -\frac{3e^2}{4\pi}k_{\rm F}.$$

This means that the ground-state energy per particle up to first-order correction is given by

$$\frac{E}{N} \approx \frac{3}{5}\left(\frac{\hbar^2 k_{\rm F}^2}{2m}\right) - \frac{3e^2}{4\pi}k_{\rm F}.$$

* Further reading: Giuliani and Vignale, Ch.2.4; Fetter and Walecka, Sec.10.

2. **Fluctuation-dissipation theorem**

For an operator $\hat{A}$, consider

$$\begin{aligned} S(t-t') &= \left\langle \hat{A}(t)\hat{A}^\dagger(t')\right\rangle, \\ i\hbar\chi(t-t') &= \Theta(t-t')\left\langle \left[\hat{A}(t), \hat{A}^\dagger(t')\right]\right\rangle. \end{aligned}$$

(a) Show that

$$S(t) = \sum_m P_m \langle m| e^{\frac{i\hat{H}t}{\hbar}}\hat{A}e^{-\frac{i\hat{H}t}{\hbar}}\hat{A}^\dagger |m\rangle = \sum_{m,n} P_m e^{-i\omega_{nm}t}|A_{mn}|^2$$

where $P_m = e^{\beta(\Omega - E_m)}/Z$ is the probability for a state m and $\omega_{nm} = \omega_n - \omega_m$.

(b) Prove that there exists a connection between $S(\omega)$ which describes the fluctuation and ${\rm Im}\chi(\omega)$ which characterizes the dissipation in a system, called the *fluctuation-dissipation theorem*:

$$S(\omega) = -\frac{2\hbar}{1-e^{-\beta\hbar\omega}}{\rm Im}\chi(\omega) = -2\hbar\left[1+n_{\rm B}(\omega)\right]{\rm Im}\chi(\omega)$$

where $n_{\rm B}(\omega) = \frac{1}{e^{\beta\hbar\omega}-1}$.

* The fluctuation-dissipation theorem is quite general and a large class of experiments in which a system is subjected to a weak controllable external probe is characterized by simple correlation functions of operators at different times.

* Further reading: Coleman, Ch.9.4; Giuliani and Vignale, Ch.3.2.6.

3. **Static structure factor**

For the density operator $\hat{\rho}(\boldsymbol{q},t) = \sum_{\boldsymbol{k},\sigma}\hat{a}^\dagger_{\boldsymbol{k}-\boldsymbol{q},\sigma}\hat{a}_{\boldsymbol{k},\sigma}$, we can define

$$\begin{aligned} S(\boldsymbol{q},t-t') &= \frac{1}{N}\left\langle \hat{\rho}(\boldsymbol{q},t)\hat{\rho}(-\boldsymbol{q},t')\right\rangle, \\ i\hbar\chi(\boldsymbol{q},t-t') &= \frac{1}{V}\Theta(t-t')\left\langle \left[\hat{\rho}(\boldsymbol{q},t), \hat{\rho}(-\boldsymbol{q},t')\right]\right\rangle. \end{aligned}$$

(a) For the Coulomb interaction, show that the interaction energy per particle is given by

$$\frac{\langle \hat{V}\rangle}{N} = \frac{1}{2}\int \frac{d^d q}{(2\pi)^d} v(\boldsymbol{q})\left[S(\boldsymbol{q})-1\right]$$

where $S(\boldsymbol{q}) = S(\boldsymbol{q}, t=0)$ is called the *static structure factor*.

(b) Show that from the fluctuation-dissipation theorem, we have

$$S(\boldsymbol{q},\omega) = -\frac{2\hbar}{n}\left[1 + n_{\rm B}(\omega)\right]\mathrm{Im}\chi(\boldsymbol{q},\omega)$$

where $n = N/V$ is the density of the system.

(c) Show that at zero temperature the static structure factor is given by

$$S(\boldsymbol{q}) = -\frac{\hbar}{n}\int_0^\infty \frac{d\omega}{\pi}\mathrm{Im}\chi(\boldsymbol{q},\omega).$$

(d) Due to causality, the response function is analytic in the upper half of the complex frequency plane, thus the integration path can be changed from the real to the imaginary axis. Then show that the structure factor in (c) can be rewritten as

$$S(\boldsymbol{q}) = -\frac{\hbar}{n}\int_0^\infty \frac{d\omega}{\pi}\chi(\boldsymbol{q},i\omega).$$

$*$ Further reading: Giuliani and Vignale, Ch.3.3.5.

4. **Noninteracting response function in imaginary frequency**

Consider the Lindhard function at imaginary frequencies for a 3D electron gas with $\varepsilon_{\boldsymbol{k}} = \frac{\hbar^2 k^2}{2m}$ at zero temperature:

$$\chi_0(\boldsymbol{q},i\omega) = g_{\rm s}\int \frac{d^d k}{(2\pi)^d}\frac{f_{\boldsymbol{k}} - f_{\boldsymbol{k}+\boldsymbol{q}}}{i\hbar\omega + \varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}+\boldsymbol{q}}}.$$

(a) Show that $\chi_0(\boldsymbol{q},i\omega)$ is real and given by

$$-\frac{\chi_0(\boldsymbol{q},i\omega)}{N_0} = \frac{2}{q/k_{\rm F}}\mathrm{Re}\left[\Psi_3\left(\frac{q}{2k_{\rm F}} + \frac{i\omega}{v_{\rm F}q}\right)\right]$$

where N_0 is the density of states (per unit volume) at the Fermi energy,

$$\Psi_3(z) = \frac{1}{2}\int_0^1 \tilde{k}^2 d\tilde{k}\int_{-1}^1 d\cos\theta\,\frac{1}{\tilde{k}\cos\theta + z} = zF(z)$$

and

$$F(z) = \frac{1}{2} - \frac{z^2-1}{4z}\ln\left(\frac{z+1}{z-1}\right).$$

(b) Prove that for $z = \frac{\tilde{q}}{2} + i\tilde{\omega}$ with real $\tilde{q}$ and $\tilde{\omega}$,

$$\ln\left(\frac{z+1}{z-1}\right) = \frac{1}{2}\ln\left|\frac{\left(\frac{\tilde{q}}{2}+1\right)^2 + \tilde{\omega}^2}{\left(\frac{\tilde{q}}{2}-1\right)^2 + \tilde{\omega}^2}\right| + i\left[\tan^{-1}\left(\frac{\tilde{\omega}}{\frac{\tilde{q}}{2}+1}\right) - \tan^{-1}\left(\frac{\tilde{\omega}}{\frac{\tilde{q}}{2}-1}\right)\right].$$

Note that the complex logarithm $\ln z = \ln|z| + i\mathrm{Arg}(z)$ is defined with the branch cut along the negative real axis so that $\mathrm{Arg}(z)$ takes the value between $-\pi$ and π.

(c) Show that finally, we have $-\chi_0(\boldsymbol{q}, i\omega)/N_0 = g\left(\frac{q}{k_\mathrm{F}}, \frac{i\omega}{v_\mathrm{F} q}\right)$ where

$$g(\tilde{q}, i\tilde{\omega}) = \frac{1}{2} + \frac{1 - \frac{\tilde{q}^2}{4} + \tilde{\omega}^2}{4\tilde{q}} \ln\left|\frac{\left(\frac{\tilde{q}}{2}+1\right)^2 + \tilde{\omega}^2}{\left(\frac{\tilde{q}}{2}-1\right)^2 + \tilde{\omega}^2}\right| + \frac{\tilde{\omega}}{2}\left[\tan^{-1}\left(\frac{\tilde{\omega}}{\frac{\tilde{q}}{2}+1}\right) - \tan^{-1}\left(\frac{\tilde{\omega}}{\frac{\tilde{q}}{2}-1}\right)\right].$$

(d) Draw $-\chi_0(\boldsymbol{q}, i\omega)/N_0$ map for $0 < q/k_\mathrm{F} < 3$ and $0 < \hbar\omega/\varepsilon_\mathrm{F} < 3$.

∗ The equation in (c) is the main expression of the noninteracting response function in imaginary frequencies for the 3D electron gas. This will be used to calculate the correlation energy. Note that $\chi_0(\boldsymbol{q}, i\omega)$ is a smooth real function thus easier to handle than $\chi_0(\boldsymbol{q}, \omega)$. Compare the map in (d) with that of $-\mathrm{Im}\left[\chi_0(\boldsymbol{q}, \omega)/N_0\right]$ in Problem 2(h) of Project 1.

∗ Further reading: Giuliani and Vignale, Ch.5.3.6; Altland and Simons, Ch.5.2 and Eq.5.30.

5. **Exchange and correlation energies of electron gas**

(a) Let's consider a Hamiltonian with a variable coupling constant λ as

$$\hat{H}_\lambda = \hat{H}_0 + \lambda\hat{V}.$$

Then show that the total energy $E = E_{\lambda=1}$ is given by

$$E = E_0 + \int_0^1 \frac{d\lambda}{\lambda} \langle\Omega_\lambda| \lambda\hat{V} |\Omega_\lambda\rangle$$

where $E_0 = \langle\Omega_0| \hat{H}_0 |\Omega_0\rangle$ and $|\Omega_\lambda\rangle$ is the ground-state of $\hat{H}_\lambda$.

(b) From the perturbation theory, the first-order correction to the ground-state energy is given by the expectation value of $\hat{V}$ in the noninteracting ground-state, $\Delta E^{(1)} = \langle\Omega_0| \hat{V} |\Omega_0\rangle$. For the Coulomb interaction in a homogeneous electron gas, $\Delta E^{(1)} = E_\mathrm{ex}$ is known as the exchange energy. Using the result of Prob. 3, show that

$$\frac{E_\mathrm{ex}}{N} = \frac{1}{2}\int \frac{d^d q}{(2\pi)^d} v(\boldsymbol{q}) \left[-\frac{\hbar}{n}\int_0^\infty \frac{d\omega}{\pi}\chi_0(\boldsymbol{q}, i\omega) - 1\right].$$

(c) Using the result of (b), draw the exchange energy per particle in units of the Rydberg energy for a 3D electron gas as a function of r_s for $0 < r_s < 20$. Compare the result with that of Problem 1.

∗ For the definition of the r_s parameter, see Problem 4 of Project 1.

(d) The remaining higher order correction is called the *correlation energy* defined by $E_\mathrm{corr} = E - E_0 - \Delta E^{(1)}$. Show that the correlation energy can be expressed as the integration over the density response function as follows:

$$\frac{E_\mathrm{corr}}{N} = -\frac{\hbar}{2n}\int \frac{d^d q}{(2\pi)^d} v(\boldsymbol{q}) \int_0^\infty \frac{d\omega}{\pi}\int_0^1 d\lambda \left[\chi_\lambda(\boldsymbol{q}, i\omega) - \chi_0(\boldsymbol{q}, i\omega))\right].$$

(e) In RPA, $\chi_\lambda(\boldsymbol{q}, i\omega) = \frac{\chi_0(\boldsymbol{q}, i\omega)}{1-\lambda v(\boldsymbol{q})\chi_0(\boldsymbol{q}, i\omega)}$. Show that the correlation energy in RPA is given by

$$\begin{aligned} \frac{E_{\rm corr}^{\rm RPA}}{N} &= \frac{\hbar}{2n}\int\frac{d^dq}{(2\pi)^d}\int_0^\infty\frac{d\omega}{\pi}\left[v(\boldsymbol{q})\chi_0(\boldsymbol{q}, i\omega) + \ln\left(1 - v(\boldsymbol{q})\chi_0(\boldsymbol{q}, i\omega)\right)\right] \\ &= \frac{\hbar}{2n}\int\frac{d^dq}{(2\pi)^d}\int_0^\infty\frac{d\omega}{\pi}\left[1 - \epsilon_{\rm RPA}(\boldsymbol{q}, i\omega) + \ln\epsilon_{\rm RPA}(\boldsymbol{q}, i\omega)\right] \end{aligned}$$

where $\epsilon_{\rm RPA}(\boldsymbol{q}, i\omega) = 1 - v(\boldsymbol{q})\chi_0(\boldsymbol{q}, i\omega)$.

(f) Draw the correlation energy per particle in units of the Rydberg energy for a 3D electron gas as a function of r_s for $0 < r_s < 20$.

$*$ Further reading: Giuliani and Vignale, Ch.1.8.3 and Ch.5.3.6, and see Fig.5.11.

References

[1] G. F. Giuliani and G. Vignale, *Quantum theory of the electron liquid*, Cambridge University Press (2005).

[2] A. Fetter and J. Walecka, *Quantum theory of many-particle systems*, Dover (2003).

[3] A. Altland and B. Simons, *Condensed matter field theory* (2nd ed.), Cambridge University Press (2010).

[4] Piers Coleman, *Introduction to Many-Body Physics*, Cambridge University Press (2016).