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Group study: Linear response theory

Project 1: Plasmon dispersion

Consider the density response to a scalar potential $v_{\rm ext}$ that couples linearly to the density $\hat{\rho}$. Then the external perturbation is given by

$$\hat{V}_{\rm ext}(t) = \int d\boldsymbol{x}\ \hat{\rho}(\boldsymbol{x},t) v_{\rm ext}(\boldsymbol{x},t).$$

Up to first order in $\hat{V}_{\rm ext}$, the density-density response function is given by

$$\delta \langle \hat{\rho}(\boldsymbol{x},t)\rangle = \int d\boldsymbol{x}' \int dt' \chi(\boldsymbol{x},t,\boldsymbol{x}',t') v_{\rm ext}(\boldsymbol{x}',t'),$$

where $\delta \langle \hat{\rho}(\boldsymbol{x},t)\rangle = \langle \hat{\rho}(\boldsymbol{x},t)\rangle_{\rm ext} - \langle \hat{\rho}(\boldsymbol{x},t)\rangle$ and

$$i\hbar\chi(\boldsymbol{x},t,\boldsymbol{x}',t') = \Theta(t-t')\left\langle [\hat{\rho}(\boldsymbol{x},t), \hat{\rho}(\boldsymbol{x}',t')]\right\rangle.$$

1. **Noninteracting response function: Derivation**

   Consider a homogeneous noninteracting electron gas in d dimensions.

   (a) Show that

$$\begin{aligned} i\hbar\chi_0(\boldsymbol{q},t) &= \frac{\Theta(t)}{V}\sum_{\boldsymbol{k},\sigma}\sum_{\boldsymbol{k}',\sigma'}\left\langle \left[\hat{a}^\dagger_{\boldsymbol{k}'-\boldsymbol{q},\sigma'}\hat{a}_{\boldsymbol{k}',\sigma'} e^{i(\omega_{\boldsymbol{k}'-\boldsymbol{q}}-\omega_{\boldsymbol{k}'})t}, \hat{a}^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma}\hat{a}_{\boldsymbol{k},\sigma}\right]\right\rangle \\ &= \frac{\Theta(t)}{V}\sum_{\boldsymbol{k},\sigma}\left\langle \hat{a}^\dagger_{\boldsymbol{k},\sigma}\hat{a}_{\boldsymbol{k},\sigma} - \hat{a}^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma}\hat{a}_{\boldsymbol{k}+\boldsymbol{q},\sigma}\right\rangle e^{i(\omega_{\boldsymbol{k}}-\omega_{\boldsymbol{k}+\boldsymbol{q}})t}. \end{aligned}$$

   (b) After Fourier transformation with respect to time, obtain

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

   where $f_{\boldsymbol{k}} = \left[e^{\beta(\varepsilon_{\boldsymbol{k}}-\mu)}+1\right]^{-1}$ is the Fermi distribution function, $g_{\rm s}=2$ is the spin degeneracy factor, and η is a positive infinitesimal number.

   (c) Explain the reason why η is necessary, and discuss the relation between causality and analytic properties of the response function.

   (d) From now on, assume that the energy spectrum is isotropic, $\varepsilon_{\boldsymbol{k}} = \varepsilon_{|\boldsymbol{k}|}$. Show that the density of states (per unit volume) at the Fermi energy $\varepsilon_{\rm F}$ is given by

$$N_0 \equiv g_{\rm s}\int \frac{d^dk}{(2\pi)^d}\delta(\varepsilon_{\boldsymbol{k}} - \varepsilon_{\rm F}) = g_{\rm s}\frac{\Omega_d}{(2\pi)^d}\frac{k_{\rm F}^{d-1}}{\hbar v_{\rm F}}$$

   where $k_{\rm F}$ is the Fermi wave vector, $v_{\rm F}$ is the Fermi velocity and $\Omega_d = \int d\Omega_d$ is the angular part of the d-dimensional integral. What is Ω_d for $d=1,2,3$?

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(e) Show that we can rearrange the equation in (b) as

$$\begin{aligned}\chi_0(\boldsymbol{q},\omega) &= -g_s \int \frac{d^dk}{(2\pi)^d} f_{\boldsymbol{k}} \left[\frac{1}{\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}} + \hbar\omega^+} + \frac{1}{\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}} - \hbar\omega^+}\right] \\ &= -\frac{N_0}{q/k_F}\left[\Psi_d\left(\frac{q}{k_F}, \frac{\omega^+}{v_F q}\right) + \Psi_d\left(\frac{q}{k_F}, -\frac{\omega^+}{v_F q}\right)\right]\end{aligned}$$

where $\omega^+ = \omega + i\eta$. The function $\Psi_d(\tilde{k}, \pm\tilde{\omega})$ is defined by

$$\Psi_d(\tilde{q}, \pm\tilde{\omega}^+) = \int_0^\infty \tilde{k}^{d-1} d\tilde{k} f_{\tilde{k}} \int \frac{d\Omega_d}{\Omega_d} \frac{1}{\Delta_{\tilde{q}}(\tilde{k}) \pm \tilde{\omega}^+},$$

where $\tilde{k} = k/k_F$, $\tilde{q} = q/k_F$, $\tilde{\omega} = \omega/v_F q$ and $\Delta_{\tilde{q}}(\tilde{k}) = \frac{\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}}}{\hbar v_F q}$. Here $\tilde{\omega}^+ = \tilde{\omega} + i\tilde{\eta}$ where $\tilde{\eta}$ is a (dimensionless) positive infinitesimal number.

$*$ Further reading: Giuliani and Vignale, Ch.4.3 and Ch. 4.4.

2. **Noninteracting response function: Analytic form**

Consider a 3D electron gas with $\varepsilon_{\boldsymbol{k}} = \frac{\hbar^2 k^2}{2m}$ at zero temperature. Let us define $-\chi_0(\boldsymbol{q},\omega)/N_0 \equiv g\left(\frac{q}{k_F}, \frac{\omega}{v_F q}\right)$.

(a) Show that

$$\Psi_3(\tilde{q}, \pm\tilde{\omega}^+) = \frac{1}{2}\int_0^1 \tilde{k}^2 d\tilde{k} \int_{-1}^1 d\cos\theta \frac{1}{\tilde{k}\cos\theta + \frac{\tilde{q}}{2} \pm \tilde{\omega}^+}.$$

(b) Show that

$$\frac{1}{2}\int_0^1 x^2 dx \int_{-1}^1 d\mu \frac{1}{x\mu + z} = zF(z)$$

where $F(z)$ is the Lindhard function defined by

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

(c) Assuming real z, draw $F(z)$ and $\frac{\partial F(z)}{\partial z}$ numerically as a function of z for $0 < z < 2$.

$*$ Note that $\frac{\partial F(z)}{\partial z}$ is singular at $z = 1$ (or $q = 2k_F$ with $\omega = 0$), which has some physical implications such as the Friedel oscillations.

(d) Prove that for real x,

$$\begin{aligned}\mathrm{Arg}(x + i\eta) &= \pi\left[1 - \Theta(x)\right], \\ \mathrm{Im}\left[\ln\frac{x+1+i\eta}{x-1+i\eta}\right] &= -\pi\Theta(1-x^2),\end{aligned}$$

where η is a positive infinitesimal number, thus we have

$$F(x \pm i\eta) = \frac{1}{2} - \frac{x^2-1}{4x}\left[\ln\left|\frac{x+1}{x-1}\right| \mp i\pi\Theta(1-x^2)\right].$$

(e) Using the results of (b) and (c), show that $\Psi_3(\tilde{q}, \pm\tilde{\omega}^+)$ in (a) is reduced to

$$\Psi_3(\tilde{q}, \pm\tilde{\omega}^+) = \nu_\pm F(\nu_\pm) \pm i\pi \frac{\nu_\pm^2 - 1}{4} \Theta(1 - \nu_\pm^2),$$

where $\nu_\pm = \frac{\tilde{q}}{2} \pm \tilde{\omega}$.

(f) Show that finally, we have

$$\begin{aligned} g(\tilde{q}, \tilde{\omega}) &= \frac{1}{2} - \frac{\nu_+^2 - 1}{4\tilde{q}} \ln\left|\frac{\nu_+ + 1}{\nu_+ - 1}\right| - \frac{\nu_-^2 - 1}{4\tilde{q}} \ln\left|\frac{\nu_- + 1}{\nu_- - 1}\right| \\ &+ i\frac{\pi}{4\tilde{q}} \left[(\nu_+^2 - 1)\Theta(1 - \nu_+^2) - (\nu_-^2 - 1)\Theta(1 - \nu_-^2)\right]. \end{aligned}$$

∗ This is the main expression of the noninteracting response function of 3D electron gas. This will be used to calculate the interacting response function and plasmon dispersion, and more.

(g) Draw $-\mathrm{Im}\left[\chi_0(\boldsymbol{q}, \omega)/N_0\right]$ map for $0 < q/k_\mathrm{F} < 3$ and $0 < \hbar\omega/\varepsilon_\mathrm{F} < 3$.

(h) In (g), there is a region within which $\mathrm{Im}\left[\chi_0(\boldsymbol{q}, \omega)\right]$ is non-zero, which is called the electron-hole continuum. Take the imaginary part of the equation in Prob. 1(b) using the relation $\mathrm{Im}\left[\frac{1}{x+i\eta}\right] = -\pi\delta(x)$, and find the boundary of the electron-hole continuum. Explain that the electron-hole continuum is directly related to the electron-hole pair excitations.

∗ Further reading: Giuliani and Vignale, Ch.4.4.

3. **Noninteracting response function: Asymptotic form**

Consider a 3D electron gas with $\varepsilon_{\boldsymbol{k}} = \frac{\hbar^2 k^2}{2m}$ at zero temperature, as in Prob. 2.

(a) In the static ($\omega \to 0$) limit, show that

$$g(\tilde{q}, \tilde{\omega} \to 0) \approx F\left(\frac{\tilde{q}}{2}\right) + i\frac{\pi}{2}\tilde{\omega}\Theta\left(1 - \frac{\tilde{q}}{2}\right) \xrightarrow{\tilde{q} \to 0} 1 - \frac{\tilde{q}^2}{12} + i\frac{\pi}{2}\tilde{\omega}.$$

∗ This expression can be used for the static screening.

(b) In the long wavelength ($|\boldsymbol{q}| \to 0$) limit, show that

$$g(\tilde{q} \to 0, \tilde{\omega} \to \infty) \approx -\frac{1}{3\tilde{\omega}^2} - \frac{1}{5\tilde{\omega}^4}.$$

∗ This expression will be used for the long wavelength plasmon dispersion.

(c) Find the plasmon dispersion in the long wavelength limit for the electron gas in 3D. (You can define the Thomas-Fermi wave vector q_TF in 3D, and express the q-corrections with q/q_TF.)

∗ Further reading: Giuliani and Vignale, Ch.4.4.3 and Ch.5.3.3.

4. **Plasmon dispersion: Numerical calculation**

The frequency and the lifetime of collective modes are determined by the poles of the retarded density correlation function. In the random phase approximation (RPA), $\chi^\mathrm{RPA}(\boldsymbol{q}, \omega) = \chi_0(\boldsymbol{q}, \omega)/\epsilon^\mathrm{RPA}(\boldsymbol{q}, \omega)$ and the Lindhard function $\chi_0(\boldsymbol{q}, \omega)$ has no poles (but only a branch cut along the real axis). Thus the poles of $\chi^{\text{RPA}}(\boldsymbol{q},\omega)$ arises from the vanishing of the dielectric function $\epsilon^{\text{RPA}}(\boldsymbol{q},\omega) = 0$.

(a) In a 3D electron gas, the r_s parameter, which plays a role of the interaction coupling constant, is defined from $\frac{4}{3}(r_s a_{\text{B}})^3 n = 1$ where n is the electron density and a_{B} is the Bohr radius with a characteristic length scale $r_s a_{\text{B}}$. For $r_s = 2$ and $q = 0.2k_{\text{F}}$, draw the real and imaginary parts of the dielectric function obtained within the RPA, $\epsilon^{\text{RPA}}(\boldsymbol{q},\omega) = 1 - v_{\text{C}}(\boldsymbol{q})\chi_0(\boldsymbol{q},\omega)$ as a function of ω for $0 < \hbar\omega/\varepsilon_{\text{F}} < 2$.

(b) For $r_s = 2$, draw the plasmon dispersion for a 3D electron gas. Along with the numerical result, draw the corresponding asymptotic form in the long wavelength limit obtained in Prob. 3(c) and add the boundary of the electron-hole continuum.

(c) Find the critical wave vector numerically where the plasmon dispersion enters into the electron-hole continuum. Note that the electron-hole continuum is defined by the region within which $\text{Im}\left[\chi_0(\boldsymbol{q},\omega)\right]$ is non-zero. See Prob. 2(h) for the discussion of the electron-hole continuum.

$*$ Further reading: Giuliani and Vignale, Ch.5.3.3 and Fig.5.8.

5. **Loss function**

(a) Show that the dielectric function and the interacting response function are related as

$$\frac{1}{\epsilon(\boldsymbol{q},\omega)} = 1 + v(\boldsymbol{q})\chi(\boldsymbol{q},\omega).$$

(b) The loss function is defined by $-\text{Im}\left[\frac{1}{\epsilon(\boldsymbol{q},\omega)}\right]$, which describes electronic energy dissipation through electron-hole pair excitations or plasmon excitations. For $r_s = 2$, draw the loss function within the RPA in logarithmic scale (or $\log_{10}\left\{-\text{Im}\left[\frac{1}{\epsilon(\boldsymbol{q},\omega)}\right]\right\}$) for $0 < q/k_{\text{F}} < 3$ and $0 < \hbar\omega/\epsilon_{\text{F}} < 3$. Along with the loss function, add the boundary of the electron-hole continuum.

(c) Find the region that the loss function is large, and explain the source of the energy dissipation.

$*$ To capture the plasmon contribution which occurs at $\epsilon(\boldsymbol{q},\omega) = 0$, add a small imaginary number $i\eta$ in $\epsilon(\boldsymbol{q},\omega)$, say $\eta = 10^{-4}$. Otherwise, the loss function will give infinity along the plasmon dispersion, which is not appropriate in numerical calculations.

$*$ Further reading: For the electron-hole continuum, see Giuliani and Vignale, Ch.4.4.2.

References

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