Condensed Matter - HW 7 :: Charged Fermi Liquid

PHSX 545

Problem 1 Yukawa potential

Find the spatial dependence of Yukawa potential $\Phi(\mathbf{r})$ in 3D. In Fourier space it is given by (k_0 is a fixed wavenumber):

$$\Phi(\mathbf{k}) = \frac{4\pi Q}{k^2 + k_0^2}$$

Find the differential equation that $\Phi(\mathbf{r})$ satisfy. (Recall the Coulomb law and its Fourier representation.)

Problem 2 Hartree-Fock

The Coulomb interactions in a conductive material have three components, electron-electron, electron-ion, ion-ion, that can be written in terms of field operators for electrons $\hat{\Psi}$ and ions $\hat{\Phi}$:

$$\hat{\mathcal{V}} = \hat{\mathcal{V}}_{ee} + \hat{\mathcal{V}}_{ei} + \hat{\mathcal{V}}_{ii}$$

$$\hat{\mathcal{V}}_{ee} = \frac{1}{2}\int d\mathbf{r} \int d\mathbf{r}' \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r}')\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\hat{\Psi}(\mathbf{r}')\hat{\Psi}(\mathbf{r})$$

$$\hat{\mathcal{V}}_{ii} = \frac{1}{2}\int d\mathbf{r} \int d\mathbf{r}' \hat{\Phi}^\dagger(\mathbf{r})\hat{\Phi}^\dagger(\mathbf{r}')\frac{Z^2e^2}{|\mathbf{r}-\mathbf{r}'|}\hat{\Phi}(\mathbf{r}')\hat{\Phi}(\mathbf{r})$$

$$\hat{\mathcal{V}}_{ei} = \int d\mathbf{r} \int d\mathbf{r}' \hat{\Psi}^\dagger(\mathbf{r})\hat{\Phi}^\dagger(\mathbf{r}')\frac{-Ze^2}{|\mathbf{r}-\mathbf{r}'|}\hat{\Phi}(\mathbf{r}')\hat{\Psi}(\mathbf{r})$$

In evaluating the contribution of Coulomb interaction to the total energy one sometimes uses the Hartree-Fock approximation.

(a) The Hartree term consists of evaluating the ensemble average $\langle\hat{\mathcal{V}}\rangle$ by pairing up creation-annihilation operators with the same arguments:

$$\langle\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})\rangle = n_e(\mathbf{r}) \qquad \text{- number density of electrons at point } \mathbf{r}$$

$$\langle\hat{\Phi}^\dagger(\mathbf{r})\hat{\Phi}(\mathbf{r})\rangle = n_i(\mathbf{r}) \qquad \text{- number density of ions at point } \mathbf{r}$$

so that the electron-electron interaction term, for example, becomes

$$V_{ee}^H = \frac{1}{2}\int d\mathbf{r} \int d\mathbf{r}' \langle\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})\rangle\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\langle\hat{\Psi}^\dagger(\mathbf{r}')\hat{\Psi}(\mathbf{r}')\rangle = \frac{1}{2}\int d\mathbf{r}\int d\mathbf{r}'\; n_e(\mathbf{r})\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}n_e(\mathbf{r}')$$

Using local (i.e. at each point $\mathbf{r}$) charge neutrality, show that the total Hartree term is zero in homogeneous gas: $V_{ee}^H + V_{ei}^H + V_{ii}^H = 0$.

(b) The Fock term, also called the exchange term, is obtained by pairing up the creation and annihilation operators at different locations (as a result there is a minus sign from the single exchange of fermionic operators):

$$V_{ee}^F = -\frac{1}{2}\int d\mathbf{r}\int d\mathbf{r}' \langle\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r}')\rangle\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\langle\hat{\Psi}^\dagger(\mathbf{r}')\hat{\Psi}(\mathbf{r})\rangle = -\frac{1}{2}\sum_{\mathbf{k},\mathbf{q}} n_{\mathbf{k}}\frac{4\pi e^2}{q^2}n_{\mathbf{k}+\mathbf{q}}\,,$$

where we went to momentum space using decomposition into plane wave basis, and introduced Fermi-Dirac distribution $\langle\hat{a}_{\mathbf{k}}^\dagger\hat{a}_{\mathbf{p}}\rangle = \delta_{\mathbf{kp}}n_{\mathbf{k}}$. Calculate the electron self-energy in ideal gas with the *unscreened* interaction at $T=0$,

$$\Sigma(k) = -\sum_{\mathbf{q}}\frac{4\pi e^2}{q^2}n_{\mathbf{k}+\mathbf{q}}\,, \quad \text{that effectively 'renormalizes' quasiparticle energy} \quad \xi(k)\to\xi'(k)=\xi(k)+\Sigma(k)$$

in the mean-field approximation, and show that it leads to unphysical infinite velocity $v_g = \partial_k\xi'(k)$ of quasiparticles at Fermi surface (which means zero effective mass, and zero DoS at Fermi level!).

Answer of exercise 1

The Fourier transform into real space is

$$\Phi(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} e^{-i\mathbf{kr}} \frac{4\pi Q}{k^2 + k_0^2} = \frac{1}{(2\pi)^3} 2\pi \int\limits_{-1}^{+1} d\cos\theta \int\limits_{0}^{\infty} k^2 dk e^{-ikr\cos\theta} \frac{4\pi Q}{k^2 + k_0^2}$$

Take the angle integral first,

$$= \frac{1}{(2\pi)^2} \int\limits_{0}^{\infty} k^2 dk \frac{e^{ikr} - e^{-ikr}}{ikr} \frac{4\pi Q}{k^2 + k_0^2} = \Big| \text{ in second exponent do } k \to -k \text{ substitution } \Big| = \frac{4\pi Q}{ir(2\pi)^2} \int\limits_{-\infty}^{\infty} kdk \frac{e^{ikr}}{k^2 + k_0^2}$$

Completing the integration contour in the UHP of comlpex-k, we go around a single pole, $k^* = ik_0$:

$$= \frac{4\pi Q}{ir(2\pi)^2} 2\pi i \frac{ik_0 e^{i(ik_0)r}}{2ik_0} = \boxed{\frac{Q}{r} e^{-k_0 r}}$$

To derive the equation satisfied by the Yukawa potential, we apply Laplacian to the integral

$$\boldsymbol{\nabla}^2 \Psi(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} \boldsymbol{\nabla}^2_{\mathbf{r}} e^{-i\mathbf{kr}} \frac{4\pi Q}{k^2 + k_0^2} = -\int \frac{d^3k}{(2\pi)^3} e^{-i\mathbf{kr}} k^2 \frac{4\pi Q}{k^2 + k_0^2} = -\int \frac{d^3k}{(2\pi)^3} e^{-i\mathbf{kr}} \left(4\pi Q - k_0^2 \frac{4\pi Q}{k^2 + k_0^2}\right)$$

add and subtract k_0^2 from k^2:

$$= -\int \frac{d^3k}{(2\pi)^3} e^{-i\mathbf{kr}} (k^2 + k_0^2 - k_0^2) \frac{4\pi Q}{k^2 + k_0^2} = -\int \frac{d^3k}{(2\pi)^3} e^{-i\mathbf{kr}} \left(4\pi Q - k_0^2 \frac{4\pi Q}{k^2 + k_0^2}\right)$$

The first part of this integral is a delta-function and the second part is the original potential:

$$\boldsymbol{\nabla}^2 \Phi(\mathbf{r}) = -4\pi Q \delta(\mathbf{r}) + k_0^2 \Phi(\mathbf{r}) \qquad \Rightarrow \qquad \boxed{(\boldsymbol{\nabla}^2 - k_0^2)\Phi(\mathbf{r}) = -4\pi Q \delta(\mathbf{r})}$$

Answer of exercise 2

(a) The total Hartree term is

$$\langle\hat{\mathcal{V}}\rangle^{Hartree} = \langle\hat{\mathcal{V}}_{ee}+\hat{\mathcal{V}}_{ei}+\hat{\mathcal{V}}_{ii}\rangle^{Hartree} = \frac{1}{2}\int d\mathbf{r}\int d\mathbf{r}'\; n_e(\mathbf{r})\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}n_e(\mathbf{r}')$$

$$+\int d\mathbf{r}\int d\mathbf{r}'\; n_e(\mathbf{r})\frac{-Ze^2}{|\mathbf{r}-\mathbf{r}'|}n_i(\mathbf{r}')+\frac{1}{2}\int d\mathbf{r}\int d\mathbf{r}'\; n_i(\mathbf{r})\frac{Z^2e^2}{|\mathbf{r}-\mathbf{r}'|}n_i(\mathbf{r}')$$

After symmetrizing the electron-ion term with respect to $\mathbf{r},\mathbf{r}'$, we can combine the three integrals into one:

$$\langle\hat{\mathcal{V}}\rangle^{Hartree} = \frac{1}{2}\int d\mathbf{r}\int d\mathbf{r}'\;[n_e(\mathbf{r})-Zn_i(\mathbf{r})]\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}[n_e(\mathbf{r}')-Zn_i(\mathbf{r}')] = 0$$

since for electrically neutral uniform system we have

$$N_e = ZN_i \qquad \Rightarrow \qquad n_e(\mathbf{r}) = Zn_i(\mathbf{r})$$

(b) The Fock or exchange self-energy is

$$\Sigma(k) = -\sum_{\mathbf{q}}\frac{4\pi e^2}{q^2}n_{\mathbf{k}+\mathbf{q}} = -\sum_{\mathbf{p}}\frac{4\pi e^2}{|\mathbf{p}-\mathbf{k}|^2}n_{\mathbf{p}}$$

At zero energy we sum over $p<p_f$ only:

$$\Sigma(k) = -\int\limits_{p<p_f}\frac{d^3p}{(2\pi)^3}\frac{4\pi e^2}{p^2+k^2-2pk\cos\theta} = \Big|u=\cos\theta\Big| = -\frac{2e^2}{2\pi}\int\limits_{-1}^{+1}du\int\limits_{0}^{p_f}\frac{p^2dp}{p^2+k^2-2pku}$$

Integrate over u first,

$$\Sigma(k) = -\frac{e^2}{2\pi k}\int\limits_0^{p_f}pdp\ln\frac{(p+k)^2}{(p-k)^2}$$

Keeping the square inside the logarythm we cover both $k>p_f$ and $k<p_f$ cases. Use the integral (theoretically minded students should take it with pen and paper, first step here is integration by parts)

$$\int xdx\ln(x+a)^2 = \frac{1}{2}\int \ln(x+a)^2\;dx^2 = \frac{1}{2}x^2\ln(x+a)^2-\int dx\frac{x^2}{x+a}$$

$$=\frac{1}{2}x^2\ln(x+a)^2-\int dx\frac{(x+a)(x-a)+a^2}{x+a} = \frac{1}{2}(x^2-a^2)\ln(x+a)^2-\left(\frac{x^2}{2}-ax\right)$$

The self-energy is

$$\Sigma(k) = -\frac{e^2}{2\pi k}\int\limits_0^{p_f}pdp\ln\frac{(p+k)^2}{(p-k)^2} = -\frac{e^2}{2\pi k}\left[\frac{1}{2}(p^2-k^2)\ln\frac{(p+k)^2}{(p-k)^2}+2kp\right]\Bigg|_{p=0}^{p=p_f} = -\frac{2e^2p_f}{\pi}F\left(\frac{k}{p_f}\right)$$

where we defined function

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

This is Lindhard function: a continuous function, including $x=1$ point, but the first derivative is divergent at that point, $F'(x=1)=-\infty$. This means that the group velocity of particles $v_g=\partial_k[\xi(k)+\Sigma(k)]$ with $k=p_f$ is infinite!