Advanced Quantum Mechanics

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Lecture #18

Quantum Mechanics of Many Particles

Recap of Last Class

Free Fermi Gas and Fermi Sea

Excitations : Particles and Holes

Interactions and Particle-Hole Excitations

Perturbation Theory for Coulomb Gas: Hartree and Fock Terms

Coulomb Gas: 1st Order Perturbation Theory

The Exchange or Fock Contribution

$$\Delta E^{(1)} = \langle\psi|H_1|\psi\rangle = r_s \sum_{kk'q\sigma\sigma'} \frac{1}{q^2} \langle\psi|c^\dagger_{k\sigma} c^\dagger_{k'\sigma'} c_{k'+q\sigma'} c_{k-q\sigma}|\psi\rangle \quad = \sum_k \Sigma(k) n_{k\sigma}$$

$$\Sigma(k) = -\frac{r_s}{\pi^2}\left[\frac{1}{2} + \frac{1-k^2}{4k}\ln\left(\frac{|1+k|}{|1-k|}\right)\right]$$

$$\Delta E^{(1)} = -\frac{r_s}{4\pi^4}\int_0^1 k^2 dk \left[1 + \frac{1-k^2}{2k}\ln\left(\frac{|1+k|}{|1-k|}\right)\right]$$

Working out the integral $\quad \Delta E^{(1)} = -\dfrac{r_s}{8\pi^4} \quad$ This is Energy / unit volume

Energy / particle is then given by $\quad \Delta E^{(1)}/\rho = -\dfrac{3r_s}{8\pi^2}$

Negative exchange correction — electrons are farther apart and feel less Coulomb repulsion

2nd Order Perturbation Theory and divergences

Can we extend this calculation to 2nd order in pert theory?

$$\Delta E^{(2)} = - \sum_{\sigma_1..\sigma_4} \sum_{k_1..k_4;q_1,q_2} V(q_1)V(q_2) \frac{\langle \psi_0 | c^\dagger_{k_3\sigma_3} c^\dagger_{k_4\sigma_4} c_{k_4-q_1\sigma_4} c_{k_3+q_1\sigma_3} | \psi_n \rangle \langle \psi_n | c^\dagger_{k_1\sigma_1} c^\dagger_{k_2\sigma_2} c_{k_2-q_2\sigma_2} c_{k_1+q_2\sigma_2} | \psi_0 \rangle}{\epsilon_{k_1} + \epsilon_{k_2} - \epsilon_{k_1+q_2} - \epsilon_{k_2+q_2}}$$

Evidently, the particles and holes created by the first application of H_1 have to be annihilated by the 2nd application of H_1

This involves pairing up all the c^+ with c s with same momentum.

$$\langle \psi_0 | c^\dagger_{k_3\sigma_3} c^\dagger_{k_4\sigma_4} c_{k_4-q_1\sigma_4} c_{k_3+q_1\sigma_3} | \psi_n \rangle \langle \psi_n | c^\dagger_{k_1\sigma_1} c^\dagger_{k_2\sigma_2} c_{k_2-q_2\sigma_2} c_{k_1+q_2\sigma_2} | \psi_0 \rangle$$

$$\langle \psi_0 | c^\dagger_{k_3\sigma_3} c^\dagger_{k_4\sigma_4} c_{k_4-q_1\sigma_4} c_{k_3+q_1\sigma_3} | \psi_n \rangle \langle \psi_n | c^\dagger_{k_1\sigma_1} c^\dagger_{k_2\sigma_2} c_{k_2-q_2\sigma_2} c_{k_1+q_2\sigma_2} | \psi_0 \rangle$$

These pairings are not allowed, as the state $|\psi_n>$ is the G.S.

At least one of the c^+ s on the right term has to be matched with a c from the left term (or vice versa).

2nd Order Perturbation Theory and divergences

$$\Delta E^{(2)} = -\sum_{\sigma_1..\sigma_4}\sum_{k_1..k_4;q_1,q_2} V(q_1)V(q_2)\frac{\langle\psi_0|c^\dagger_{k_3\sigma_3}c^\dagger_{k_4\sigma_4}c_{k_4-q_1\sigma_4}c_{k_3+q_1\sigma_3}|\psi_n\rangle\langle\psi_n|c^\dagger_{k_1\sigma_1}c^\dagger_{k_2\sigma_2}c_{k_2-q_2\sigma_2}c_{k_1+q_2\sigma_2}|\psi_0\rangle}{\epsilon_{k_1}+\epsilon_{k_2}-\epsilon_{k_1+q_2}-\epsilon_{k_2+q_2}}$$

$$\langle\psi_0|c^\dagger_{k_3\sigma_3}c^\dagger_{k_4\sigma_4}c_{k_4-q_1\sigma_4}c_{k_3+q_1\sigma_3}|\psi_n\rangle\langle\psi_n|c^\dagger_{k_1\sigma_1}c^\dagger_{k_2\sigma_2}c_{k_2-q_2\sigma_2}c_{k_1+q_2\sigma_2}|\psi_0\rangle$$

Not allowed : $q_1=0$ will lead to $|\psi_n>$ being the G.S

Both the c^+ s on the right term has to be matched with c s from the left term (and vice versa).

$$\langle\psi_0|c^\dagger_{k_3\sigma_3}c^\dagger_{k_4\sigma_4}c_{k_4-q_1\sigma_4}c_{k_3+q_1\sigma_3}|\psi_n\rangle\langle\psi_n|c^\dagger_{k_1\sigma_1}c^\dagger_{k_2\sigma_2}c_{k_2-q_2\sigma_2}c_{k_1+q_2\sigma_2}|\psi_0\rangle$$

$k_3=k_1+q_2$ $\quad$ $k_3+q_1=k_1$ $\quad$ $q_1=-q_2$

$$\langle\psi_0|c^\dagger_{k_3\sigma_3}c^\dagger_{k_4\sigma_4}c_{k_4-q_1\sigma_4}c_{k_3+q_1\sigma_3}|\psi_n\rangle\langle\psi_n|c^\dagger_{k_1\sigma_1}c^\dagger_{k_2\sigma_2}c_{k_2-q_2\sigma_2}c_{k_1+q_2\sigma_2}|\psi_0\rangle$$

$k_3=k_2-q_2$ $\quad$ $k_3+q_1=k_2$ $\quad$ $q_1=q_2$

2nd Order Perturbation Theory and divergences

$$\Delta E^{(2)} = -\sum_{\sigma_1..\sigma_4}\sum_{k_1..k_4;q_1,q_2} V(q_1)V(q_2)\frac{\langle\psi_0|c^\dagger_{k_3\sigma_3}c^\dagger_{k_4\sigma_4}c_{k_4-q_1\sigma_4}c_{k_3+q_1\sigma_3}|\psi_n\rangle\langle\psi_n|c^\dagger_{k_1\sigma_1}c^\dagger_{k_2\sigma_2}c_{k_2-q_2\sigma_2}c_{k_1+q_2\sigma_2}|\psi_0\rangle}{\epsilon_{k_1}+\epsilon_{k_2}-\epsilon_{k_1+q_2}-\epsilon_{k_2+q_2}}$$

$$\langle\psi_0|c^\dagger_{k_3\sigma_3}c^\dagger_{k_4\sigma_4}c_{k_4-q_1\sigma_4}c_{k_3+q_1\sigma_3}|\psi_n\rangle\langle\psi_n|c^\dagger_{k_1\sigma_1}c^\dagger_{k_2\sigma_2}c_{k_2-q_2\sigma_2}c_{k_1+q_2\sigma_2}|\psi_0\rangle$$

$k_3=k_1+q_2$ $k_3+q_1=k_1$ $q_1=-q_2$

$$\langle\psi_0|c^\dagger_{k_3\sigma_3}c^\dagger_{k_4\sigma_4}c_{k_4-q_1\sigma_4}c_{k_3+q_1\sigma_3}|\psi_n\rangle\langle\psi_n|c^\dagger_{k_1\sigma_1}c^\dagger_{k_2\sigma_2}c_{k_2-q_2\sigma_2}c_{k_1+q_2\sigma_2}|\psi_0\rangle$$

$k_3=k_2-q_2$ $k_3+q_1=k_2$ $q_1=q_2$

Both terms involve an integral of the form

$$\Delta E^{(2)} \sim -r_s^2\int_0^\infty \frac{q^2dq}{q^4}\sum_{k_1k_2}F(k_1,k_2,q)$$

Infrared divergence from q=0

This comes due to the long range rature of Coulomb potential

Screening to Rescue

If an external charge distribution is placed in a medium containing charges, the response of the medium includes rearranging its own charges to lower the potential energy.

This leads to ideas of induced charges and displacement fields (D vs E) in electrodynamics.

We have been assuming that an electron is a charged particle placed in the E field of other electrons. In pert. theory we have assumed these other electrons to have the same distribution as if they are non-interacting.

We need to take into account how the charge distribution rearranges to get the correct answers. This process is non-perturbative and hence the simple pert. theory breaks down.

However, if we can treat this redistribution in some approximation, we can deal with the potential due to the redistributed charges perturbatively.

Induced Charges and Dielectric function

Consider the response of the electron gas to an externally imposed charge distribution

$$H_{ext} = \int d^3x \int d^3x' \hat{\rho}(x) V(x-x') \rho_{ext}(x',t)$$

Operator A   Control Field f(t)

Note: A - sign reqd to cast in the form H_1 = -f(t) A

The external charge distribution induces an additional charge $\rho_{ind}(x,t) = \langle \delta\hat{\rho}(x,t) \rangle$

Operator B

Define total charge $\rho_{tot}(x,t) = \rho_{ext}(x,t) + \rho_{ind}(x,t)$

For translation invariant system, F.T. to get $\rho_{tot}(q,\omega) = \rho_{ext}(q,\omega) + \rho_{ind}(q,\omega) = \dfrac{\rho_{ext}(q,\omega)}{\varepsilon(q,\omega)}$

Defines the q, ω dependent dielectric function

Our aim is to calculate ρ_{ind} within linear response theory

$$\rho_{ind}(x,t) = -\int d^3x' \int d^3x'' \int dt' \chi_{\rho\rho}(x-x', t-t') V(x'-x'') \rho_{ext}(x'',t')$$

Induced Charges and Dielectric function

Consider the response of the electron gas to an externally imposed charge distribution

$$H_{ext} = \int d^3x \int d^3x' \hat{\rho}(x) V(x-x') \rho_{ext}(x',t) \qquad \rho_{ind}(x,t) = \langle \delta\hat{\rho}(x,t) \rangle$$

Operator A   Control Field f(t)   Operator B

$$\rho_{ind}(x,t) = -\int d^3x' \int d^3x'' \int dt' \chi_{\rho\rho}(x-x', t-t') V(x'-x'') \rho_{ext}(x'',t')$$

For translation invariant system, F.T. to get

$$\rho_{ind}(q,\omega) = -\chi_{\rho\rho}(q,\omega) V(q) \rho_{ext}(q,\omega)$$

Defn. of dielectric fn. $\quad \rho_{tot}(q,\omega) = \rho_{ext}(q,\omega) + \rho_{ind}(q,\omega) = \dfrac{\rho_{ext}(q,\omega)}{\varepsilon(q,\omega)}$

$$\varepsilon^{-1}(q,\omega) = 1 - V(q)\chi_{\rho\rho}(q,\omega)$$

Dielectric function

$$\varepsilon^{-1}(q,\omega) = 1 + V(q)\chi_{\rho\rho}(q,\omega)$$

From Linear Response Theory,

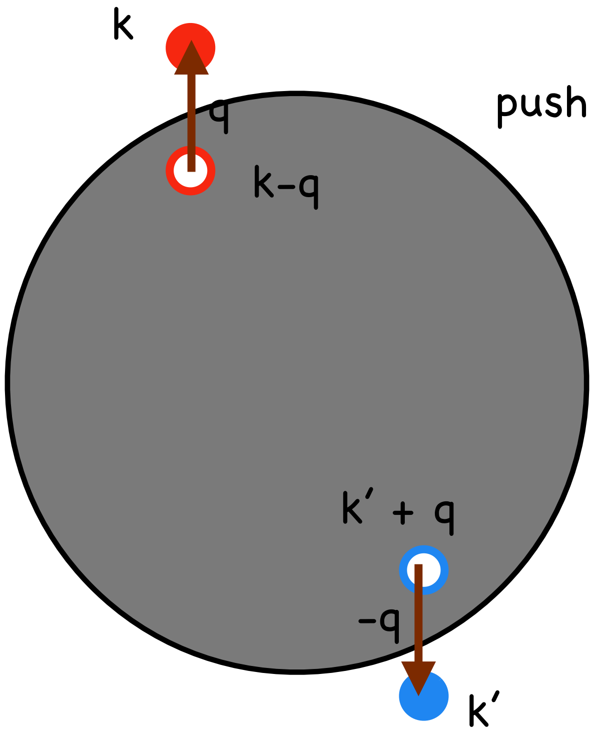
$$\chi_{\rho\rho}(q,\omega) = \sum_n \frac{2\omega_{n0}|\langle n|\hat{\rho}(q)|0\rangle|^2}{(\omega+i\eta)^2-\omega_{n0}^2}$$

$$= \sum_n \frac{\langle 0|\hat{\rho}^\dagger(q)|n\rangle\langle n|\hat{\rho}(q)|0\rangle}{(\omega+i\eta-\omega_{n0}} - \frac{\langle 0|\hat{\rho}(q)|n\rangle\langle n|\hat{\rho}^\dagger(q)|0\rangle}{(\omega+i\eta+\omega_{n0}}$$

$$\hat{\rho}(q) = \sum_{k\sigma} c^\dagger_{k+q\sigma}c_{k\sigma}$$

$$\hat{\rho}^\dagger(q) = \sum_{k\sigma} c^\dagger_{k\sigma}c_{k+q\sigma} = \sum_{k\sigma} c^\dagger_{k-q\sigma}c_{k\sigma} = \hat{\rho}(-q)$$

Particle-Hole Excitations and Interactions



Number conserving excitations:
push a Fermion from inside the FS to a momentum state outside FS

A particle with momentum k and a hole at k-q

State carries a net momentum q

Energy of the state (measured from ground state energy)

$$E = \epsilon_k - \epsilon_{k-q}$$

Effect of the Interaction term on the Fermi Sea

$$c^\dagger_{k\sigma} c^\dagger_{k'\sigma'} c_{k'+q\sigma'} c_{k-q\sigma}$$

Note: k, k′ outside FS; k-q, k′+q inside FS

2 pairs of particle-hole excitations of spin σ and σ'

State carries zero momentum

Energy of the state (measured from ground state energy) $E = \epsilon_k + \epsilon_{k'} - \epsilon_{k-q} - \epsilon_{k'+q}$

Dielectric function

$$\varepsilon^{-1}(q,\omega) = 1 - V(q)\chi_{\rho\rho}(q,\omega) \qquad \varepsilon(q,\omega) = 1 + V(q)\chi_{\rho\rho}(q,\omega)$$

From Linear Response Theory,

$$\chi_{\rho\rho}(q,\omega) = \sum_n \frac{2\omega_{n0}|\langle n|\hat{\rho}(q)|0\rangle|^2}{(\omega+i\eta)^2 - \omega_{n0}^2}$$

$$= \sum_n \frac{\langle 0|\hat{\rho}^\dagger(q)|n\rangle\langle n|\hat{\rho}(q)|0\rangle}{(\omega+i\eta-\omega_{n0})} - \frac{\langle 0|\hat{\rho}(q)|n\rangle\langle n|\hat{\rho}^\dagger(q)|0\rangle}{(\omega+i\eta+\omega_{n0})}$$

$$\hat{\rho}(q) = \sum_{k\sigma} c^\dagger_{k+q\sigma}c_{k\sigma}$$

$$\hat{\rho}^\dagger(q) = \sum_{k\sigma} c^\dagger_{k\sigma}c_{k+q\sigma} = \sum_{k\sigma} c^\dagger_{k-q\sigma}c_{k\sigma} = \hat{\rho}(-q)$$

$$\chi_{\rho\rho}(q,\omega) = \sum_k \frac{n_k(1-n_{k+q}) - (1-n_k)n_{k+q}}{(\omega+i\eta-\epsilon_{k+q}+\epsilon_k)}$$

$$= \sum_k \frac{n_k - n_{k+q}}{(\omega+i\eta-\epsilon_{k+q}+\epsilon_k)}$$

$$= \sum_k n_k \left[\frac{1}{(\omega+i\eta-\epsilon_{k+q}+\epsilon_k)} - \frac{1}{(\omega+i\eta-\epsilon_k+\epsilon_{k+q})}\right]$$

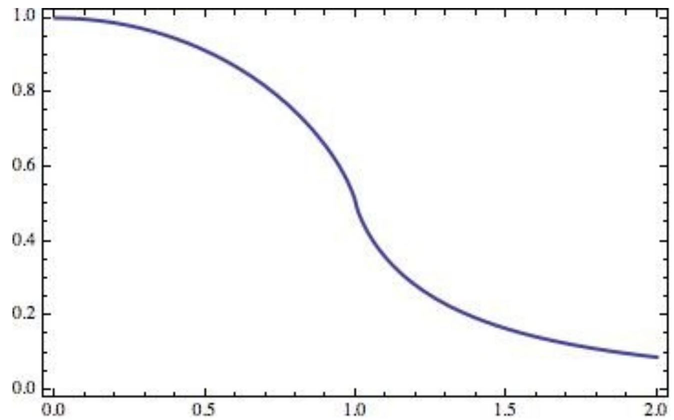
$$= \frac{1}{4\pi^2}\int_0^1 k^2 dk \int_{-1}^1 du \left[\frac{1}{(\omega+i\eta-q^2/2m-kqu/m)} - \frac{1}{(\omega+i\eta+q^2/2m-kqu/m)}\right]$$

Static RPA Screening

take ω=0 limit

$$\chi_{\rho\rho}(q,0) = \frac{1}{4\pi^2}\int_0^1 k^2 dk \int_{-1}^{1} du \left[\frac{1}{-q^2/2m - kqu/m)} - \frac{1}{(+q^2/2m - kqu/m)}\right]$$

Doing the integrals $\chi_{\rho\rho}(q,0) = \frac{mk_F}{\pi^2} u(q/2k_F)$



And hence

$$\varepsilon(q,0) = [1 + (9/4\pi)^{1/3}\frac{r_s k_F^2}{q^2} u(q/2k_F)]$$

Effective Screened Interaction $V_{eff}(q) = \frac{V(q)}{\varepsilon(q,0)} = \frac{V(q)}{1 + V(q)\chi_{\rho\rho}(q)}$

As q –> 0 u(q/2) ⟶ 1 $V_{eff}(q) \to 1/\chi_{\rho\rho}(q)$

No divergence for pert. theory with screened interaction.