561 Fall 2005 Lecture 8

The Random Phase Approximation and the consequences for the One-Electron Green's Functions

Primary references: Pines, 136-163; Mahan Ch. 2.8, 3.4, 5.5B, 5.6, 5.8; Fetter, Sec. 12. Phillips describes aspects of the RPA in Ch. 8. See p. 129, especially Eq. (8.71).

1. Screened Coulomb interaction in solids

Recall from lecture 5b that the change in the total potential inside a solid $\delta V_{total,int}$ due to an external potential δV_{ext} is given to linear order by

$$\delta V_{total,int} = \epsilon^{-1}\delta V_{ext}; \ \delta V_{ext} = \epsilon \ \delta V_{int}. \tag{1}$$

(Here the notation is changed slightly to clarify that the changes are small and that $\delta V_{total,int}$ means the total internal field including the external field. The term "external means any field acting on the electrons, which may come from the nuclei, sources outside the material, etc.)

We showed that ϵ^{-1} is closely related to the retarded density-density response function D^R defined in lecture 5. The relation is $(\epsilon^{-1}(\mathbf{k}, \omega) - 1) = \frac{4\pi e^2}{k^2}\Pi^R(\mathbf{k}, \omega)$, where $\Pi^R = \frac{\delta\rho_{int}}{\delta(V_{ext})} = \frac{1}{\hbar}D^R(\mathbf{k}, \omega)$. Finally, we showed that $\epsilon(\mathbf{k}, \omega)$ is also a response function.

The random phase approximation brings out all these features that become apparent in the expressions that can be evaluated analytically for the electron gas. Furthermore, the RPA provides a reasonable approximation to electronic correlation that removes the unphysical features found in the Hartree-Fock approximation.

2. Random Phase Approximation for screening of Coulomb Interactions, i.e., the dielectric function

A screened interaction can be written diagrammatically as:

The interaction can be written in general in the for of a Dyson's Eq.:

$$W(k, \omega) \equiv V(k)\epsilon^{-1}(k, \omega) = V(k) + V(k)\Pi^\star(k, \omega)V(k) + \ldots = \frac{V(k)}{1 - V(k)\Pi^\star(k, \omega)} \tag{2}$$

or

$$\epsilon^{-1}(k, \omega) = \frac{1}{1 - V(k)\Pi^\star(k, \omega)}, \tag{3}$$

which means that

$$\epsilon(k, \omega) = 1 - V(k)\Pi^\star(k, \omega), \tag{4}$$

where $\Pi^\star(k, \omega)$ is the proper (irreducible) polarizability or density-density correlation.

3. RPA form for the polarization self-energy $\Pi^\star_{RPA}(k, \omega)$

"RPA" means Random Phase Approximation, i.e., that each Coulomb interaction at a wavevector q is independent of other q'. This is the reason that $\Pi^\star_{RPA}(k, \omega)$ reduces to the simple "bubble" diagram shown at the bottom of the figure. The diagram corresponds to the excitation of an electron from a filled to an empty state, integrating over all such excitations.

Evaluation of the RPA approximation for the proper polarizability follows from the simple form of the "bubble". Following the rules for constructing diagrams (see Mahan

$$\text{Dyson's Eq.} \quad W(q,\omega) = \frac{V(q)}{1 - V(q)\,\Pi^*(q,\omega)}$$

RPA – neglect all internal Coulomb interaction lines with momentum ≠ q – see discussion – then

$$\Pi^*(q,\omega) =$$

Figure 1: Screened interaction. The top figures are examples of diagrams and the definition of the proper polarizability. The bottom figure show the result of the RPA - one single bubble diagram - see text.
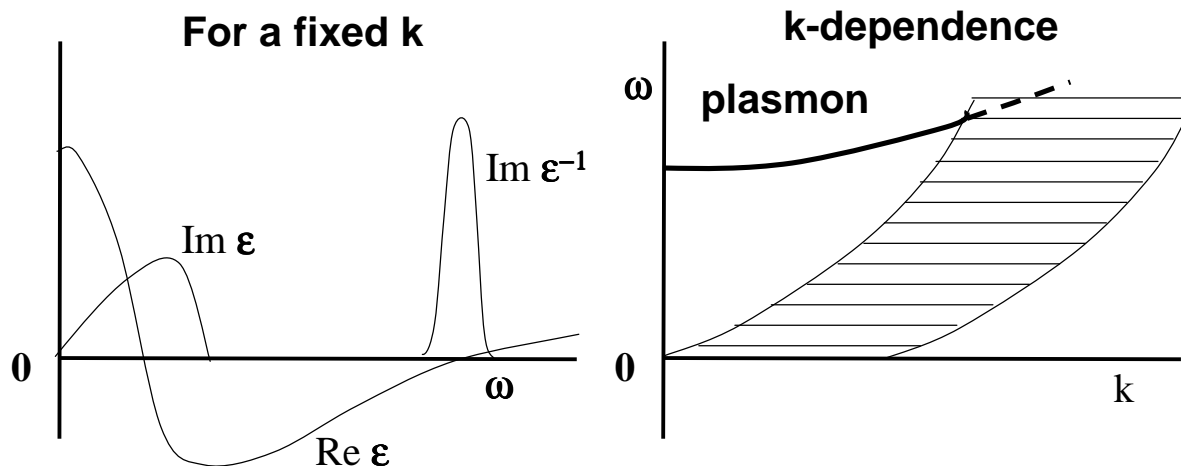
Figure 2: Schematic illustration of the real and imaginary parts of $\epsilon(k, \omega)$ and $\epsilon^{-1}(k, \omega)$ in the RPA. General features are expected to hold in the exact function, but there will be non-zero imaginary parts in at all frequencies. (Why? - question to the students.)

or Fetter) the diagram represents the product of two non-interacting G^0 Green's functions with integration over the internal variables p and E.

$$\Pi^\star_{RPA}(k, \omega) = (-i)(2) \int_{-\infty}^{\infty} dE \frac{1}{2\pi} \sum_p G^0(p, E) G^0(p + q, E + \omega), \qquad (5)$$

where the factor of 2 is for spin. Note that the G^0 functions are time-ordered and thus have poles in the upper half plane for $\epsilon(p) = p^2/2m < \mu$ and in the lower half plane for $\epsilon(p) = p^2/2m > \mu$. The integral is zero for both states p and q occupied or both states empty (because the integral can be closed encircling no poles). The integral is non-zero only if one state is filled and the other empty. Thus the time-ordered form has the correct physics automatically included.

Evaluation of the energy integral leads to (for explicit expressions see Mahan (2.8.1) and Fetter, 158):

$$\Pi^\star(k, \omega) = 2 \sum_{p,\sigma} \Theta(\epsilon_{p+k,\sigma} - \mu) \Theta(\mu - \epsilon_{p,\sigma})$$

$$\left[\frac{1}{\omega - (\epsilon_{p+k,\sigma} - \epsilon_{p,\sigma}) + i\eta} - \frac{1}{\omega + (\epsilon_{p+k,\sigma} + \epsilon_{p,\sigma}) - i\eta} \right]. \qquad (6)$$

Using the relation $\epsilon(k, \omega) = 1 - V(k)\Pi^\star(k, \omega)$,, this leads to the famous Lindhard expression for the dielectric function, given in Phillips, Pines, Mahan and many sources.

(Note - the proper definition of the dielectric function is a causal function, whereas we evaluated a time-ordered function. The correct retarded function is the same as above but with $+i\eta$ in the second term. Then all poles are in the lower half plane and one has the correct form that $Re\Pi$ is even in ω and $Im\Pi$ is odd.)

Key points:

- The imaginary part of the dielectric function is non-zero only for a finite range of ω for a given value of q. This is easy to show and will be discussed in class.

- The real part can be derived by a KK analysis.

- In a metal for $\omega \to 0$, ϵ always diverges as $k \to 0$ (take limit with $\omega \to 0$ first) which screens the Coulomb interaction and cancels the $1/k^2$ divergence.

- The real part of the dielectric function vanishes at the plasma frequency just as can be derived from simple arguments. See previous notes.

4. What is omitted in the RPA?

The key point is that the electron-hole excitations in the proper polarizability Π^* are non-interacting. All interactions of the electron and hole are omitted.

Note that the RPA includes some effects of the interaction through the average $V(q)$ in the infinite sum of diagrams in the total polarizability Π.

5. Dynamic Structure factor $S(k, \omega)$

From our notes on dielectric functions, we found the general relation for $S(k, \omega)$ in terms of the retarded Density-Density Response Function:

$$S(k, \omega) = -\frac{\hbar}{\pi} Im\Pi^{retarded}(k, \omega) = \frac{k^2}{4\pi e^2} Im(\epsilon^{-1}(k, \omega) - 1), \tag{7}$$

where $\Pi^{retarded}(k, \omega)$ is the full density-density response function. Now we have clarified that $\Pi(k, \omega)$ is an infinite series of diagrams, which can always be expressed in terms of the simpler set of proper diagrams $\Pi^\star(k, \omega)$ that cannot be cut by a single G^0 line. From knowledge of $\Pi^{\star\ retarded}(k, \omega)$ we can determine $\Pi^{retarded}(k, \omega)$ and thus the desired structure factor. Furthermore, this is the most desirable form for making approximations.

6. Comparison to Hartree-Fock expression for ϵ^{-1}

The Hartree Fock ϵ is defined so that $S(k, \omega)$ agrees with the Hartree-Fock form (see Pines, p. 136-7). This gives $\epsilon_{HF}^{-1}(k, \omega) = 1 - V(k)\Pi_{RPA}^\star(k, \omega)$, which is only the lowest order term in the expansion of the actual RPA form for ϵ^{-1}, which is an infinite series in $\Pi_{RPA}^\star$. Thus the Hartree-Fock approximation includes only the only lowest order term in the strength of the interaction e^2.

7. Ground State energy

The ground state energy can be gotten as an integral over $Im\epsilon^{-1}(k, \omega)$ as shown in Pines, Appendix C, lecture notes no. 5, and homework.

Note $E_{RPA} < E_{HF}$ as it must if RPA includes correlations beyond HF. (This is opposite to what one gets with statically screened exchange, which lowers the magnitude of the exchange energy, i.e., it increases the total energy.)

8. One-electron Green's function Beyond Hartree-Fock

The most obvious problem with H-F is that it leads to a self-energy $\Sigma_k^\star$ that is independent of energy E; in jellium it varies too rapidly with k is singular at $k = k_F$, and the singularity must occur is any metal. . The only way the singularity can be eliminated is for the exchange to be screened for k near k_F (and E near E_F).
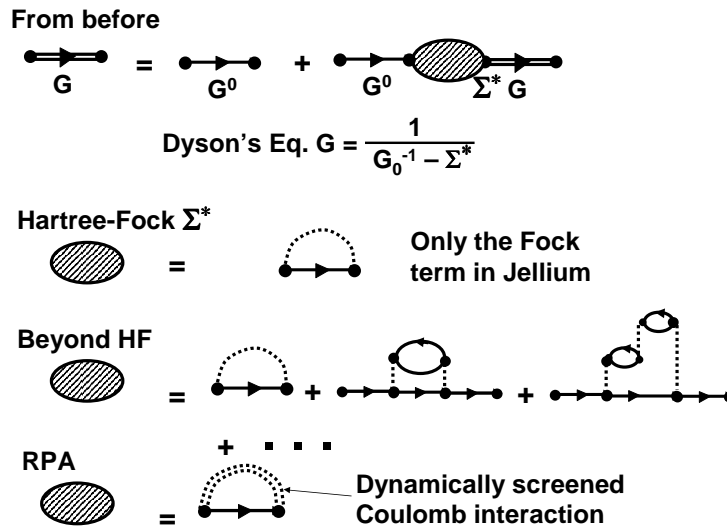
From before

Dyson's Eq. $G = \dfrac{1}{G_0^{-1} - \Sigma^*}$

Hartree-Fock Σ^*

Only the Fock term in Jellium

Beyond HF

RPA

Dynamically screened Coulomb interaction

Figure 3: Electron self-energy $\Sigma^*_{RPA}(k, E)$ in the RPA. (This is ofte called the "GW" approximation because it represents a single diagram with an electron Green's function G and an RPA screened interaction W.
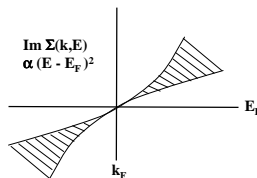

Figure 4: Schematic illustration of the peak in the Green's function, with width $\propto Im\Sigma^\star_\lambda(E)$, just as described in the previous notes.

RPA focuses on the screening of the interaction and leads to a consistent theory that eliminates the worst problems. The key is the self-energy concept *applied to the interaction.*

9. Key results
Quasiparticles are well-defined near E_{Fermi}
RPA screens the HF exchange at low energies
Lifetime is finite; $Im\Sigma^\star(E) \propto E^2$
This is guaranteed by phase space factors, so long as 1) the effective screened Coulomb interaction for excitations near the Fermi energy is short range and 2) the perturbation theory converges.
Dispersion, weights of quasiparticle energies modified
Weights Z reduced from unity
There is a discontinuity in the momentum distribution at the Fermi surface, but the step size is reduced.
Total energy improved over Hartree-Fock
Since the RPA is frequency dependent, it does not screen the Coulomb interaction at high

frequencies, and it even increases the attractive exchange interaction.

The energy is lower than Hartree-Fock; in fact it is too low, as shown by essentially exact calculations.

Experiments: Tunnelling, photoemission, scattering
Examples discussed in class.