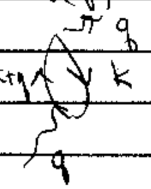
6/4/03

Last gasps....

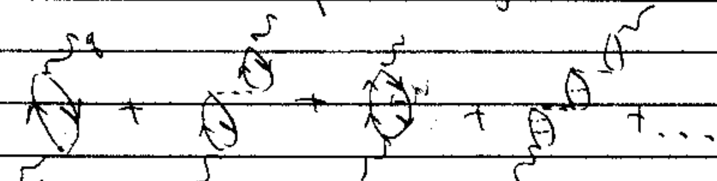
RPA in pictures:

- We considered the non-interacting approximation to the response function $D_0(\vec{q}, \omega)$:

$D_0(\vec{q},\omega) =$ 

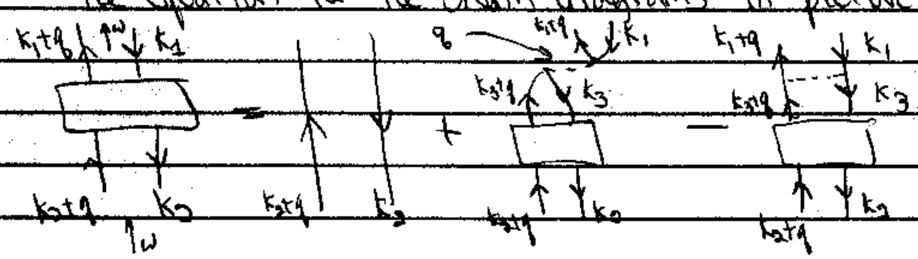
which we were able to calculate explicitly.

- For the RPA, we want to sum up the rings and ladders: "chain diagrams"

$D_{RPA}(\vec{q},\omega) =$ 

We can do this most directly by opening the vertices connecting to the external perturbation, so that we are dealing with the "particle-hole" Green's function, which is a special case of the general four-point (or two-particle) Green's function.

- The equation for the chain diagrams in pictures is:



- The boxes on the right are the same as the one on the left.
- By iterating this equation, we precisely generate the sum of chain diagrams with open ends. At the end we can close the ends and we have D_{RPA}. (we sum over k_1 and k_2).

6/4/03

We can see that the potential in the direct term only depends on the momentum transfer $\vec{q}$, so we get the Fourier transform of the potential $\tilde{V}(-\vec{q})$ [or a constant if it is a delta function interaction].

· If we just include the direct terms, we find (in Negele/Orland notation):

$$\boxed{G^{RPA}(k_1+q, k_1 | k_2+q, k_2; \omega) = G_0^{ph}(k_1; q, \omega)\left[\delta_{k_1 k_2} + \frac{\tilde{V}(\vec{q})\, G_0^{ph}(k_2; q, \omega)}{1-\tilde{V}(q) D_0(q,\omega)}\right]}$$

where

$$\boxed{G_0^{ph}(k, q; \omega) = \frac{(1-n_{k+q})\, n_k}{\omega+\epsilon_k-\epsilon_{k+q}+i\eta} - \frac{(1-n_k)\, n_{k+q}}{\omega+\epsilon_k-\epsilon_{k+q}-i\eta}}$$

particles

holes

$k+q$ k

and

$$\boxed{D_0(\vec{q},\omega) = \sum_{\vec{k}} G_0^{ph}(k; q, \omega)}$$

$k+q$ k

· We find $\boxed{D^{RPA}(q,\omega) = \sum_{k_1,k_2} G^{RPA}(k_1+q, k_1 | k_2+q, k_2; \omega)}$

· Since the excited states are found by looking at the poles of D^{RPA} (or G^{RPA}) in ω, we see that these occur when

$$\boxed{\tilde{V}(\vec{q})\, D_0(q,\omega) = 1}$$

· For fixed $\vec{q}$, if $\vec{k}$ is in the Fermi sea and $\vec{k+q}$ is outside, then there is a pole in $D_0(q,\omega)$ when $\omega = \epsilon_{k+q}-\epsilon_k$. For a repulsive potential then, $D_0(q,\omega)$ as a function of ω goes to $+\infty$ or $-\infty$ at these ω's (depending on whether approaching from above or below) and is a decreasing function in between.

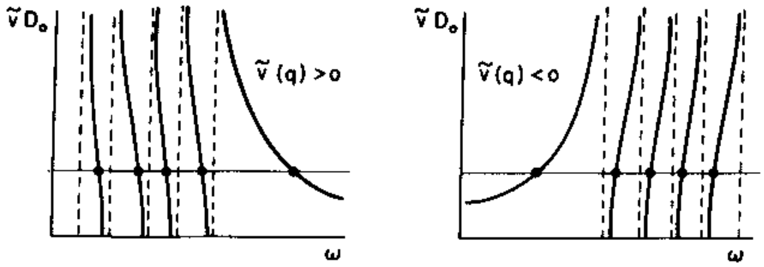


Fig. 5.13 Graphical solution for the RPA modes. The vertical asymptotes correspond to the particle-hole excitations $\omega = \epsilon_{k+q} - \epsilon_q$ and the curves **show the qualitative behavior of $\tilde{v}(q)D_0(q,\omega)$ for the repulsive and attractive potentials, respectively.**

The qualitative behavior of $\tilde{v} D_0$ is shown by the solid lines in the figure. The straight line is 1 and the intersections are the desired poles in ω of $D^{RPA}(q,\omega)$.

Note that they lie between the "unperturbed" energies except for one state that is pushed up (repulsive) or down (attractive). The latter are the collective states.

- An example in a electron gas (Coulomb force) is the plasmon. (see Negele and Orland, pp 269-270.)

Sum Rules

Consider the integral of $\operatorname{Im} D(x_1, x_2; \omega)$ over ω:

$$\int d\omega \operatorname{Im} D(\vec{x}_1, \vec{x}_2; \omega) = -\pi \sum_n \int d\omega\, \delta(\omega - E_n^N + E_0^N)$$

$$\times \langle \Psi_0^N | \hat{\rho}(\vec{x}_1) - \langle \hat{\rho}(\vec{x}_1) \rangle | \Psi_n^N \rangle \langle \Psi_n^N | \hat{\rho}(\vec{x}_2) - \langle \hat{\rho}(\vec{x}_2) \rangle | \Psi_0^N \rangle$$

$$= -\pi \langle \Psi_0^N | (\hat{\rho}(\vec{x}_1) - \langle \hat{\rho}(\vec{x}_1) \rangle)(\hat{\rho}(\vec{x}_2) - \langle \hat{\rho}(\vec{x}_2) \rangle) | \Psi_0^N \rangle$$

$$= -\pi \left[\langle \Psi_0^N | \hat{\rho}(\vec{x}_1) \hat{\rho}(\vec{x}_2) | \Psi_0^N \rangle - \langle \hat{\rho}(\vec{x}_1) \rangle \langle \hat{\rho}(\vec{x}_2) \rangle \right]$$

$$= -\pi \left[\langle \rho(\vec{x}_1) \rho(\vec{x}_2) \rangle - \langle \rho(\vec{x}_1) \rangle \langle \rho(\vec{x}_2) \rangle \right]$$

$$= -\pi \left[g(\vec{x}_1, \vec{x}_2) + \delta(\vec{x}_1 - \vec{x}_2) \rho(\vec{x}_1) \right]$$

where $g(\vec{x}_1, \vec{x}_2)$ is the two-body correlation function:

$$g(\vec{x}_1, \vec{x}_2) \equiv \langle \Psi_0^N | \hat{\psi}^\dagger(\vec{x}_1) \hat{\psi}^\dagger(\vec{x}_2) \hat{\psi}(\vec{x}_2) \hat{\psi}(\vec{x}_1) | \Psi_0^N \rangle - \langle \Psi_0^N | \hat{\rho}(\vec{x}_1) | \Psi_0^N \rangle \langle \Psi_0^N | \hat{\rho}(\vec{x}_2) | \Psi_0^N \rangle$$

In uniform systems, $\boxed{g(\vec{x}_1, \vec{x}_2) = g(\vec{x}_1 - \vec{x}_2)}$

and

$$\boxed{S(q) \equiv -\frac{1}{\pi N} \int d\omega \operatorname{Im} D(q, \omega) = \rho \int d^3x\, e^{-iq\cdot x} g(x) + 1}$$

so measuring $\operatorname{Im} D(q,\omega)$ in inclusive scattering gives us the Fourier transform of the two-body correlation function.

An example for ^{4}He is on the next page.

6/4/03

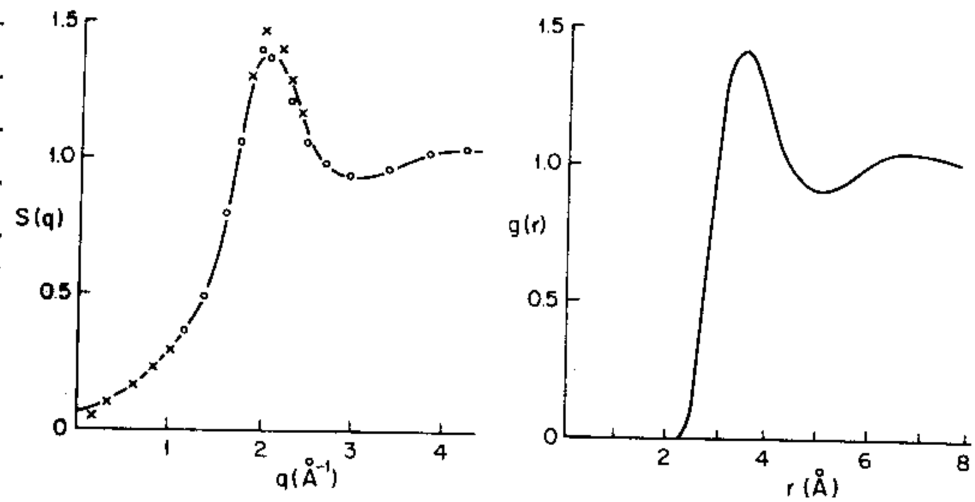


Fig. 5.18 Liquid structure function $S(q)$ and two-body correlation function $g(r)$ for liquid ^{4}He. The left-hand graph compares X-ray scattering data of Hallock (1972) and Rubkoff *et al.* (1979) (crosses) and neutron scattering data of Svensson *et al.* (1980) (circles) with the structure function obtained from Monte Carlo calculations (solid curves) of Kalos *et al.* (1981). The right-hand graph shows the two-body correlation function corresponding to this $S(q)$.

Various sum rules can be derived by calculating the ground state expectation value of double commutators.

For example, considering $[[\hat{H}, \hat{\rho}_q], \hat{\rho}_{-q}]$ yields

$$\boxed{-\frac{1}{\pi N}\int d\omega\, \omega \,\mathrm{Im}\, D(q,\omega) = \frac{q^2}{2m}}$$

and if $\hat{D}$ is the electric dipole moment operator of a nucleus relative to the COM, then the general sum rule

$$\boxed{\langle \Psi_0^N | [\hat{D},[\hat{H},\hat{D}]] | \Psi_0^N \rangle = \sum_n (E_n - E_0) |\langle \Psi_n^N | \hat{D} | \Psi_0^N \rangle|^2}$$

becomes $\boxed{4\sum_n (E_n - E_0) |\langle \Psi_n^N | \hat{D} | \Psi_0^N \rangle|^2 = \frac{6\hbar^2 NZ}{mA}}$ For N neutrons, Z protons, $A = Z + N$

"Giant" dipole resonance states exhausts large fraction of sum rule!