The Random Phase Approximation (RPA): example of the retarded density-density correlation function

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We have seen that two-particle correlation functions naturally emerge in the linear-response formalism. An example is the retarded density-density correlation function

$$\chi^R(\vec{r}t, \vec{r}'t') = -i\theta(t-t')\langle[\rho(\vec{r}t), \rho(\vec{r}'t')]\rangle$$

which we have already evaluated in the special case of a non-interacting electron gas. In the interacting case, the corresponding function can be obtained in the random phase approximation (RPA), which gives a decent description of interacting Fermi gases. The RPA will be used in the framework of the equation-of-motion approach, where it provides the means to decouple the higher order Green's functions that show up in the equation of motion for χ^R.

The decoupling procedure is inspired by the Hartree-type mean-field approach to interacting systems. Consider a system with the Hamiltonian $\boxed{H = H_0 + V_{int}}$, where

$$H_0 = \sum_\nu \xi_\nu c_\nu^\dagger c_\nu \quad ; \quad V_{int} = \frac{1}{2}\sum_{\nu\nu'} V_{\nu\mu,\nu'\mu'} c_\nu^\dagger c_\mu^\dagger c_{\mu'} c_{\nu'}$$

Then we can write $c_\nu^\dagger c_\mu^\dagger c_{\mu'} c_{\nu'}$ as

$$c_\nu^\dagger c_\mu^\dagger c_{\mu'} c_{\nu'} = c_\nu^\dagger\left(c_\mu^\dagger c_{\mu'} - \langle c_\mu^\dagger c_{\mu'}\rangle\right)c_{\nu'} + c_\nu^\dagger c_{\nu'}\langle c_\mu^\dagger c_{\mu'}\rangle \Rightarrow$$

If the quantum number ν' is different from μ, we can commute $c_{\nu'}$ with the parentheses and get

$$c_\nu^\dagger c_\mu^\dagger c_{\mu'} c_{\nu'} \cong c_\nu^\dagger c_{\nu'}\left(c_\mu^\dagger c_{\mu'} - \langle c_\mu^\dagger c_{\mu'}\rangle\right) + c_\nu^\dagger c_{\nu'}\langle c_\mu^\dagger c_{\mu'}\rangle.$$

If we now also write $c_\nu^\dagger c_{\nu'}$ as

$$c_\nu^\dagger c_{\nu'} = c_\nu^\dagger c_{\nu'} - \langle c_\nu^\dagger c_{\nu'} \rangle + \langle c_\nu^\dagger c_{\nu'} \rangle$$

and insert it into the last equation, we get:

$$\underline{\underline{c_\nu^\dagger c_\mu^\dagger c_{\mu'} c_{\nu'}}} \simeq \left(c_\nu^\dagger c_{\nu'} - \langle c_\nu^\dagger c_{\nu'} \rangle \right) \left(c_\mu^\dagger c_{\mu'} - \langle c_\mu^\dagger c_{\mu'} \rangle \right)$$
$$+ \langle c_\nu^\dagger c_{\nu'} \rangle \left(c_\mu^\dagger c_{\mu'} - \langle c_\mu^\dagger c_{\mu'} \rangle \right)$$
$$+ c_\nu^\dagger c_{\nu'} \langle c_\mu^\dagger c_{\mu'} \rangle$$
$$\simeq \boxed{\langle c_\nu^\dagger c_{\nu'} \rangle c_\mu^\dagger c_{\mu'} + c_\nu^\dagger c_{\nu'} \langle c_\mu^\dagger c_{\mu'} \rangle - \langle c_\nu^\dagger c_{\nu'} \rangle \langle c_\mu^\dagger c_{\mu'} \rangle}$$

where the term $\left(c_\nu^\dagger c_{\nu'} - \langle c_\nu^\dagger c_{\nu'} \rangle \right) \left(c_\mu^\dagger c_{\mu'} - \langle c_\mu^\dagger c_{\mu'} \rangle \right)$ can be dropped on the grounds of being small.

The equation-of-motion approach works for two-particle correlation functions in a way similar to the single-particle Green's functions. If $C_{AB}^R(t,t') \equiv -i\theta(t-t') \langle [A(t), B(t')] \rangle$ then

$$i\partial_t C_{AB}^R(t,t') = i(-i)\, \partial_t \theta(t-t') \langle [A(t), B(t')] \rangle$$
$$\Leftrightarrow \qquad -i\theta(t-t') \langle [i\partial_t A(t), B(t')] \rangle$$

$$\boxed{\begin{aligned} i\partial_t C_{AB}^R(t,t') &= \delta(t-t') \langle [A(t), B(t')] \rangle \\ (*) \qquad & + i\theta(t-t') \langle [[H,A](t), B(t')] \rangle \end{aligned}}$$

where we made use of the fact that $\boxed{i\partial_t A(t) = -[H,A](t)}$.

The Hamiltonian of the system is given by

$$H = \underbrace{\sum_{\vec{k}} \xi_{\vec{k}} c^{+}_{\vec{k}} c_{\vec{k}}}_{H_0} + \underbrace{\frac{1}{2\nu} \sum_{\vec{k},\vec{k}',\vec{q}} V(q)\, c^{+}_{\vec{k}+\vec{q}}\, c^{+}_{\vec{k}'-\vec{q}}\, c_{\vec{k}'} c_{\vec{k}}}_{V_{int}}$$

ν – volume of the system

In the last Hamiltonian we ignored the spin degree of freedom, since the latter is irrelevant for the present discussion.

As we have already seen, after a spatial Fourier transformation $\chi^R(\vec{r}t, \vec{r}t')$ becomes

$$\chi^R(\vec{q}, t-t') = -\frac{i}{\nu}\,\theta(t-t') \langle [\rho(\vec{q},t), \rho(-\vec{q},t')] \rangle$$

where $\rho(\vec{q}) = \sum_{\vec{k}} c^{+}_{\vec{k}} c_{\vec{k}+\vec{q}}$ is the Fourier transform of the density operator.

[Note that $\rho = \rho^{+}$ implies that $\rho(\vec{q}) = \rho^{+}(\vec{q}) = \rho(-\vec{q})$, a property that we will need in the forthcoming derivation!]

As it turns out, it is more convenient to carry out derivations with the correlation function

$$\chi^R(\vec{k}\vec{q}, t-t') \equiv -i\,\theta(t-t') \langle [c^{+}_{\vec{k}} c_{\vec{k}+\vec{q}}(t), \rho(-\vec{q},t')] \rangle$$

and then obtain $\chi^R(\vec{q}, t-t')$ as

$$\boxed{\chi^R(\vec{q}, t-t') = \frac{1}{\nu} \sum_{\vec{k}} \chi^R(\vec{k}\vec{q}, t-t')}$$

Thus by benefiting from the already derived Eq. (*) for $A(t) \equiv c^{+}_{\vec{k}} c_{\vec{k}+\vec{q}}(t)$ and $B(t') \equiv \rho(-\vec{q}, t')$ we get

$$i \partial_t \chi^R(\vec{k}\vec{q}, t-t') = \delta(t-t') \left\langle \left[c^{+}_{\vec{k}} c_{\vec{k}+\vec{q}}(t), \rho(-\vec{q}, t') \right] \right\rangle$$
$$+ i \theta(t-t') \left\langle \left[\left[H, c^{+}_{\vec{k}} c_{\vec{k}+\vec{q}}(t) \right], \rho(-\vec{q}, t') \right] \right\rangle$$

Using the well-known identity

$$[c_m^{+} c_n, c_p^{+} c_q] = \delta_{np} c_m^{+} c_q - \delta_{mq} c_p^{+} c_n ,$$

we obtain $\left[c^{+}_{\vec{k}} c_{\vec{k}+\vec{q}}, \rho(-\vec{q}) \right] = \sum_{\vec{k}'} \left[c^{+}_{\vec{k}} c_{\vec{k}+\vec{q}}, c^{+}_{\vec{k}'} c_{\vec{k}'-\vec{q}} \right] =$

$$= c^{+}_{\vec{k}} c_{\vec{k}} - c^{+}_{\vec{k}+\vec{q}} c_{\vec{k}+\vec{q}}$$

and $\left[H_0, c^{+}_{\vec{k}} c_{\vec{k}+\vec{q}} \right] = (\xi_{\vec{k}} - \xi_{\vec{k}+\vec{q}}) c^{+}_{\vec{k}} c_{\vec{k}+\vec{q}}$,

while two subsequent applications of the same identity yield

$$\left[V_{int}, c^{+}_{\vec{k}} c_{\vec{k}+\vec{q}} \right] = \frac{1}{2V} \sum_{\vec{k}'\vec{q}'} V(q') \Big\{ c^{+}_{\vec{k}+\vec{q}'} c^{+}_{\vec{k}'-\vec{q}'} c_{\vec{k}'} c_{\vec{k}+\vec{q}} +$$
$$+ c^{+}_{\vec{k}'+\vec{q}'} c^{+}_{\vec{k}-\vec{q}'} c_{\vec{k}+\vec{q}} c_{\vec{k}'} - c^{+}_{\vec{k}'+\vec{q}} c^{+}_{\vec{k}} c_{\vec{k}+\vec{q}+\vec{q}'} c_{\vec{k}'} -$$
$$- c^{+}_{\vec{k}} c^{+}_{\vec{k}'-\vec{q}} c_{\vec{k}'} c_{\vec{k}+\vec{q}-\vec{q}'} \Big\} .$$

Using the decoupling prescription described at the beginning of this lecture, we obtain

$$\left[V_{int}, c^\dagger_{\vec k} c_{\vec k+\vec q}\right] \overset{RPA}{\approx} \frac{1}{2V} \sum_{\vec k', \vec q' \neq 0} V(q') \Big\{ \langle c^\dagger_{\vec k+\vec q'} c_{\vec k+\vec q} \rangle c^\dagger_{\vec k'-\vec q'} c_{\vec k'}$$

$$+ c^\dagger_{\vec k+\vec q'} c_{\vec k+\vec q} \langle c^\dagger_{\vec k'-\vec q'} c_{\vec k'} \rangle$$

$$+ \langle c^\dagger_{\vec k'+\vec q'} c_{\vec k'} \rangle c^\dagger_{\vec k-\vec q'} c_{\vec k+\vec q}$$

$$+ c^\dagger_{\vec k'+\vec q'} c_{\vec k'} \langle c^\dagger_{\vec k-\vec q'} c_{\vec k+\vec q} \rangle$$

$$- \langle c^\dagger_{\vec k'+\vec q'} c_{\vec k'} \rangle c^\dagger_{\vec k} c_{\vec k+\vec q+\vec q'}$$

$$- c^\dagger_{\vec k'+\vec q'} c_{\vec k'} \langle c^\dagger_{\vec k} c_{\vec k+\vec q+\vec q'} \rangle$$

$$- \langle c^\dagger_{\vec k} c_{\vec k+\vec q-\vec q'} \rangle c^\dagger_{\vec k'-\vec q'} c_{\vec k'}$$

$$- \langle c^\dagger_{\vec k'-\vec q'} c_{\vec k'} \rangle c^\dagger_{\vec k} c_{\vec k+\vec q-\vec q'} \Big\}$$

Using the fact that

$$\langle c^\dagger_{\vec k} c_{\vec k'} \rangle \equiv \langle n_{\vec k} \rangle \delta_{\vec k, \vec k'}$$

we can easily see that from the eight terms obtained only four are nonzero (since $\vec q' \neq 0$)

$$\Downarrow$$

$$\left[V_{int}, c^\dagger_{\vec k} c_{\vec k+\vec q}\right] \overset{RPA}{\approx} \frac{1}{2V} \sum_{\vec k', \vec q'} V(q') * \Big\{ \langle n_{\vec k+\vec q} \rangle \delta_{\vec q', \vec q} c^\dagger_{\vec k'-\vec q} c_{\vec k'}$$

$$+ \langle n_{\vec k+\vec q} \rangle \delta_{\vec q', -\vec q} c^\dagger_{\vec k'+\vec q} c_{\vec k'}$$

$$- \langle n_{\vec k} \rangle \delta_{\vec q', -\vec q} c^\dagger_{\vec k'+\vec q} c_{\vec k'}$$

$$- \langle n_{\vec k} \rangle \delta_{\vec q', \vec q} c^\dagger_{\vec k'-\vec q} c_{\vec k'} \Big\} =$$

$$= \frac{1}{2V} \left(\langle n_{\vec k+\vec q} \rangle - \langle n_{\vec k} \rangle \right) \Big\{ V(q) \sum_{\vec k'} c^\dagger_{\vec k'-\vec q} c_{\vec k'} + V(-q) \sum_{\vec k'} c^\dagger_{\vec k'+\vec q} c_{\vec k'} \Big\}$$

Now note that $\sum_{\vec k'} c^\dagger_{\vec k'-\vec q} c_{\vec k'} \equiv \sum_{\vec k'} c^\dagger_{\vec k'} c_{\vec k'+\vec q} \equiv \rho(\vec q)$ and that $\sum_{\vec k'} c^\dagger_{\vec k'+\vec q} c_{\vec k'} \equiv \sum_{\vec k'} c^\dagger_{\vec k'} c_{\vec k'-\vec q} \equiv \rho(-\vec q)$, but as we already showed $\rho(-\vec q) = \rho(\vec q)$! $\Longrightarrow$

Since we also have that $V(-q) = V(q)$ for the Coulomb potential (in fact, this will be true for any spherically-symmetric potential!), we have

$$\boxed{\left[V_{int},\, c^{\dagger}_{\vec{k}}\, c_{\vec{k}+\vec{q}}\right] \overset{RPA}{\approx} \frac{1}{\mathcal{V}}\left(\langle n_{\vec{k}+\vec{q}}\rangle - \langle n_{\vec{k}}\rangle\right) V(q)\, \rho(\vec{q})}$$

With the derived commutators the equation of motion for $\chi^R(\vec{k}\vec{q}, t-t')$ becomes

$$i\partial_t \chi^R(\vec{k}\vec{q}, t-t') = \delta(t-t')\left(\langle n_{\vec{k}}\rangle - \langle n_{\vec{k}+\vec{q}}\rangle\right)$$

$$+ \left(\xi_{\vec{k}} - \xi_{\vec{k}+\vec{q}}\right) * i\,\theta(t-t')\left\langle\left[c^{\dagger}_{\vec{k}}\, c_{\vec{k}+\vec{q}}(t),\, \rho(-\vec{q}, t')\right]\right\rangle$$

$$+ \frac{1}{\cancel{\mathcal{V}}}\left(\langle n_{\vec{k}+\vec{q}}\rangle - \langle n_{\vec{k}}\rangle\right) V(q) * \underbrace{i\,\theta(t-t')\left\langle\left[\rho(\vec{q}, t),\, \rho(-\vec{q}, t')\right]\right\rangle}_{\to -\cancel{\mathcal{V}}\,\chi^R(\vec{q},\, t-t')}$$

$$\Longleftrightarrow \quad \left(i\partial_t + \xi_{\vec{k}} - \xi_{\vec{k}+\vec{q}}\right)\chi^R(\vec{k}\vec{q}, t-t') =$$

$$= \left(\langle n_{\vec{k}}\rangle - \langle n_{\vec{k}+\vec{q}}\rangle\right)\left[\delta(t-t') + V(q)\,\chi^R(\vec{q}, t-t')\right],$$

which after Fourier transformation in time becomes

$$\boxed{\begin{aligned} &\left(\omega + \xi_{\vec{k}} - \xi_{\vec{k}+\vec{q}} + i\eta\right)\chi^R(\vec{k}, \vec{q}, \omega) \\ &\quad = \left(\langle n_{\vec{k}}\rangle - \langle n_{\vec{k}+\vec{q}}\rangle\right)\left[1 + V(q)\,\chi^R(\vec{q}, \omega)\right] \end{aligned}},$$

$\eta \to 0^+$

that is

$$\chi^R(\vec{k}\vec{q},\omega) = \frac{\langle n_{\vec{k}}\rangle - \langle n_{\vec{k}+\vec{q}}\rangle}{\omega + \xi_{\vec{k}} - \xi_{\vec{k}+\vec{q}} + i\eta}\left[1 + V(q)\chi^R(\vec{q},\omega)\right]$$

$$\Downarrow$$

recall that $\langle n_{\vec{k}}\rangle \equiv n_F(\xi_{\vec{k}})$ at $T=0$

$$\left[\frac{1}{V}\sum_{\vec{k}}\chi^R(\vec{k}\vec{q},\omega) = \underbrace{\frac{1}{V}\sum_{\vec{k}}\frac{\langle n_{\vec{k}}\rangle - \langle n_{\vec{k}+\vec{q}}\rangle}{\omega + \xi_{\vec{k}} - \xi_{\vec{k}+\vec{q}} + i\eta}}_{\equiv\, \chi_0^R(\vec{q},\omega)}\left[1 + V(q)\chi^R(\vec{q},\omega)\right]\right]$$

Lindhard's function

$$\Leftrightarrow \quad \chi^R(\vec{q},\omega) = \chi_0^R(\vec{q},\omega)\left[1 + V(q)\chi^R(\vec{q},\omega)\right] \Leftrightarrow$$

$$\chi^R(\vec{q},\omega)\left[1 - V(q)\chi_0^R(\vec{q},\omega)\right] = \chi_0^R(\vec{q},\omega) \Rightarrow$$

$$\boxed{\chi^R(\vec{q},\omega) = \frac{\chi_0^R(\vec{q},\omega)}{1 - V(q)\chi_0^R(\vec{q},\omega)}}$$

This is the <u>RPA polarization function.</u>

The <u>RPA dielectric function</u> is given by

$$\varepsilon^{RPA}(\vec{q},\omega) = \left[1 + V(q)\chi^R(\vec{q},\omega)\right]^{-1}, \text{ that is,}$$

$$\varepsilon^{RPA}(\vec{q},\omega) = \frac{1}{1 + V(q)\dfrac{\chi_0^R(\vec{q},\omega)}{1 - V(q)\chi_0^R(\vec{q},\omega)}} \Rightarrow$$

$$\Leftrightarrow \quad \boxed{\varepsilon^{RPA}(\vec{q},\omega) = 1 - V(q)\chi_0^R(\vec{q},\omega)}$$