

On the equilibrium two particle Wigner distribution  
function for an electron gas.

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ABSTRACT :

We present here an expression for the equilibrium two particle Wigner distribution function,  $f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q})$ , within the mean field approximation, using the equation of motion approach. We show that the modification to the non-interacting form for  $f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q})$  enters through the longitudinal dielectric function which incorporates the dielectric screening effects.

The equilibrium two particle Wigner distribution function  $f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q})$ , is a quantity that often appears in equation of motion approaches employed to study the many body effects in the homogeneous electron gas [1]. However an expression for this function, even in the simplest approximation, has not been made available so far. On the other hand, any theory based on the equation of motion for the two particle distribution function (e.g., calculation carried out recently by Aravind et al [2]) requires, as input, the form for  $f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q})$ . The aim of this paper, therefore, is to obtain an expression for  $f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q})$ . For this purpose we employ the equation of motion approach and work within the mean field approximation.

In section 1, we give definitions of some relevant quantities and enumerate certain general properties of the equilibrium function. In section 2, we describe the equation of motion approach and obtain an expression for  $f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q})$ . Finally in section 3 we discuss the implications of our result.

## 1. DEFINITIONS AND GENERAL PROPERTIES.

We begin with the definition of the non-equilibrium form for the irreducible two particle distribution function in real space, given by,

$$f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)}(\underline{r}, \underline{r}', t) = \frac{1}{V^2} \int d^3x d^3x' e^{i\underline{k}\cdot\underline{x}} e^{i\underline{k}'\cdot\underline{x}'}$$

$$\left\{ \langle \psi_{\sigma}^{\dagger}(\underline{r} + \frac{\underline{x}}{2}, t) \psi_{\sigma'}^{\dagger}(\underline{r}' + \frac{\underline{x}'}{2}, t) \psi_{\sigma}(\underline{r}' - \frac{\underline{x}'}{2}, t) \psi_{\sigma'}(\underline{r} - \frac{\underline{x}}{2}, t) \rangle - \langle \psi_{\sigma}^{\dagger}(\underline{r} + \frac{\underline{x}}{2}, t) \psi_{\sigma}(\underline{r} - \frac{\underline{x}}{2}, t) \rangle \langle \psi_{\sigma'}^{\dagger}(\underline{r}' + \frac{\underline{x}'}{2}, t) \psi_{\sigma'}(\underline{r}' - \frac{\underline{x}'}{2}, t) \rangle \right\},$$

where  $\Psi_0$  are the usual field operators for the interacting electrons of spin  $\sigma$  in a large volume  $V$ . In Fourier space, it can be expressed in terms of the usual creation and annihilation operators  $a_{\underline{k}\sigma}^+$  and  $a_{\underline{k}\sigma}$  respectively as,

$$f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)}(\underline{q}, \underline{q}', t) = \langle a_{\underline{k}-\underline{q}/2\sigma}^+(t) a_{\underline{k}'-\underline{q}'/2\sigma'}^+(t) a_{\underline{k}'+\underline{q}'/2\sigma'}(t) a_{\underline{k}+\underline{q}/2\sigma}(t) \rangle - \langle a_{\underline{k}-\underline{q}/2\sigma}^+(t) a_{\underline{k}+\underline{q}/2\sigma}(t) \rangle \langle a_{\underline{k}'-\underline{q}'/2\sigma'}^+(t) a_{\underline{k}'+\underline{q}'/2\sigma'}(t) \rangle. \quad (2)$$

In terms of the density fluctuation operators  $\hat{\rho}_{\underline{k}\sigma}(\underline{q})$ , defined as,

$$\hat{\rho}_{\underline{k}\sigma}(\underline{q}, t) = \hat{S}_{\underline{k}\sigma}(\underline{q}, t) - \langle \hat{S}_{\underline{k}\sigma}(\underline{q}, t) \rangle_{eq}, \quad (3a)$$

with,

$$\hat{S}_{\underline{k}\sigma}(\underline{q}, t) = a_{\underline{k}-\underline{q}/2\sigma}^+(t) a_{\underline{k}+\underline{q}/2\sigma}(t), \quad (3b)$$

we can rewrite (2) as,

$$f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)}(\underline{q}, \underline{q}', t) = \langle \hat{\rho}_{\underline{k}\sigma}(\underline{q}, t) \hat{\rho}_{\underline{k}'\sigma'}(\underline{q}', t) \rangle - \delta_{\sigma\sigma'} \delta_{\underline{k}', \underline{k} + \frac{\underline{q} + \underline{q}'}{2}} \langle \hat{S}_{\underline{k}+\underline{q}'/2\sigma}(\underline{q} + \underline{q}', t) \rangle. \quad (4)$$

In equilibrium, i.e., in the absence of an external field, we have,

$$\langle \hat{S}_{\underline{k}\sigma}(\underline{q}) \rangle_{eq} = n_{\underline{k}\sigma} \delta_{\underline{q}, 0}, \quad (5)$$

where  $n_{\underline{k}\sigma}$  is the single particle momentum distribution function for the interacting system. Using (5), the equilibrium two particle distribution function can be written in terms of density fluctuation operators as,

$$f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q}) = \delta_{\underline{q} + \underline{q}', 0} f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)}(\underline{q}, \underline{q}'),$$

$$= \langle \hat{\rho}_{\underline{k}\sigma}(\underline{q}) \hat{\rho}_{\underline{k}'\sigma'}(-\underline{q}) \rangle_{eq} - \delta_{\sigma\sigma'} \delta_{\underline{k}\underline{k}'} n_{\underline{k}-\underline{q}/2\sigma}, \quad (6)$$

where the first equality follows from the translational symmetry of the system. Due to rotational symmetry in

a homogeneous system, it also follows that,

$$f_{\underline{k}\sigma, \underline{k}'\sigma'}^{(2)eq}(-\underline{q}) = f_{-\underline{k}\sigma, -\underline{k}'\sigma'}^{(2)eq}(\underline{q}) \quad (7)$$

The sum over all momenta and spins, gives an exact condition,

$$\sum_{\underline{k}\sigma, \underline{k}'\sigma'} f_{\underline{k}\sigma, \underline{k}'\sigma'}^{(2)eq}(\underline{q}) = N[S(\underline{q}) - 1], \quad (8)$$

where  $S(\underline{q})$  is the usual static structure factor of the interacting electron system.

The first term on the right hand side of (6) is related to a retarded density-density response function, defined as,

$$\chi_{\underline{k}\sigma, \underline{k}'\sigma'}(\underline{q}, t) = \frac{\theta(t)}{i\hbar V} \left\langle \left[ \hat{\tilde{S}}_{\underline{k}\sigma}(\underline{q}, t), \hat{\tilde{S}}_{\underline{k}'\sigma'}(-\underline{q}, 0) \right]_- \right\rangle_{eq}, \quad (9)$$

through a relation, (details in Appendix A), which at the temperature  $T=0$ , reads,

$$\left\langle \hat{\tilde{S}}_{\underline{k}\sigma}(\underline{q}) \hat{\tilde{S}}_{\underline{k}'\sigma'}(-\underline{q}) \right\rangle_{eq} = -\frac{\hbar V}{\pi} \int_0^{\infty} d\omega \operatorname{Im} \chi_{\underline{k}\sigma, \underline{k}'\sigma'}(\underline{q}, \omega), \quad (10)$$

where  $\chi_{\underline{k}\sigma, \underline{k}'\sigma'}(\underline{q}, \omega)$  is the temporal Fourier transform of  $\chi_{\underline{k}\sigma, \underline{k}'\sigma'}(\underline{q}, t)$ . Thus the problem is reduced to obtaining an expression for the response function, which we do in the next section.

## 2. EXPRESSION FOR $f_{\underline{k}\sigma, \underline{k}'\sigma'}^{(2)eq}(\underline{q})$

We use here the equation of motion approach to first obtain  $\chi_{\underline{k}\sigma, \underline{k}'\sigma'}(\underline{q}, t)$ . From the definition (9), we have,

$$i\hbar \frac{\partial}{\partial t} \chi_{\underline{k}\sigma, \underline{k}'\sigma'}(\underline{q}, t) = \frac{\delta(t)}{V} \delta_{\underline{k}, \underline{k}'} \delta_{\sigma\sigma'} (\eta_{\underline{k}-\underline{q}/2\sigma} - \eta_{\underline{k}+\underline{q}/2\sigma}) + \frac{\theta(t)}{V} \left\langle \left[ \frac{\partial \hat{\tilde{S}}_{\underline{k}\sigma}(\underline{q}, t)}{\partial t}, \hat{\tilde{S}}_{\underline{k}'\sigma'}(-\underline{q}, 0) \right]_- \right\rangle_{eq}, \quad (11)$$

where we have used the commutation properties of the density fluctuation operators and (5) to rewrite the first term. The equation of motion for  $\hat{\rho}_{\underline{k}\sigma}(\underline{q}, t)$ , using the fully interacting Hamiltonian, is given by,

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}_{\underline{k}\sigma}(\underline{q}, t) = \frac{\hbar^2}{m} (\underline{k} \cdot \underline{q}) \hat{\rho}_{\underline{k}\sigma}(\underline{q}, t)$$

$$+ \frac{1}{V} \sum_{\underline{q}_1} v(\underline{q}_1) \hat{\rho}(\underline{q}_1, t) [\hat{\rho}_{\underline{k}-\underline{q}_1/2\sigma}(\underline{q}-\underline{q}_1, t) - \hat{\rho}_{\underline{k}+\underline{q}_1/2\sigma}(\underline{q}-\underline{q}_1, t)], \quad (12)$$

where  $v(q) (= 4\pi e^2/q^2)$  is the spatial Fourier transform of the interaction between the electrons.

Substitution of (12) in (11) leads to higher order correlations entering the equation. In the present work, we restrict ourselves to the mean field (i.e. time-ordered Hartree or RPA like) approximation and hence rewrite (12) as,

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}_{\underline{k}\sigma}(\underline{q}, t) = \frac{\hbar^2}{m} (\underline{k} \cdot \underline{q}) \hat{\rho}_{\underline{k}\sigma}(\underline{q}, t)$$

$$+ \frac{v(\underline{q})}{V} (n_{\underline{k}-\underline{q}/2\sigma} - n_{\underline{k}+\underline{q}/2\sigma}) \hat{\rho}(\underline{q}, t).$$

Substituting the above in (11) and taking its temporal Fourier transform, we have,

$$\chi_{\underline{k}\sigma \underline{k}'\sigma'}(\underline{q}, \omega) = \chi_{\underline{k}\sigma}^0(\underline{q}, \omega) \left[ \delta_{\sigma\sigma'} \delta_{\underline{k}\underline{k}'} + \frac{v(\underline{q}) \chi_{\underline{k}'\sigma'}^0(\underline{q}, \omega)}{\epsilon(\underline{q}, \omega)} \right]. \quad (13)$$

Here, we have defined,

$$\chi_{\underline{k}\sigma}^0(\underline{q}, \omega) = \frac{1}{\hbar V} \frac{(n_{\underline{k}-\underline{q}/2\sigma} - n_{\underline{k}+\underline{q}/2\sigma})}{\omega + i\delta - \frac{\hbar}{m} \underline{k} \cdot \underline{q}}, \quad (14a)$$

$$\chi^0(\underline{q}, \omega) = \sum_{\underline{k}\sigma} \chi_{\underline{k}\sigma}^0(\underline{q}, \omega), \quad (14b)$$

$$\text{and } \epsilon(\underline{q}, \omega) = 1 - v(\underline{q}) \chi^0(\underline{q}, \omega). \quad (15)$$

By definition,  $\chi^0(\underline{q}, \omega)$  is the usual Lindhard function and  $\epsilon$  has the standard RPA form for the longitudinal dielectric function.

Note that the following relations follow,

$$\sum_{\underline{k}\sigma} \chi_{\underline{k}\sigma \underline{k}'\sigma'}(\underline{q}, \omega) = \chi_{\underline{k}'\sigma'}^0(\underline{q}, \omega) / \epsilon(\underline{q}, \omega), \quad (16a)$$

$$\sum_{\underline{k}'\sigma'} \chi_{\underline{k}\sigma \underline{k}'\sigma'}(\underline{q}, \omega) = \chi_{\underline{k}\sigma}^0(\underline{q}, \omega) / \epsilon(\underline{q}, \omega), \quad (16b)$$

and,

$$\sum_{\underline{k}\sigma \underline{k}'\sigma'} \chi_{\underline{k}\sigma \underline{k}'\sigma'}(\underline{q}, \omega) = \chi^0(\underline{q}, \omega) / \epsilon(\underline{q}, \omega) \equiv \chi(\underline{q}, \omega). \quad (16c)$$

Clearly the condition (8), follows from (16), (10) and (4) with the static structure factor  $S(\underline{q})$  given by its RPA form.

Using (13) in (10) and explicitly writing the expression for the imaginary part of  $\chi_{\underline{k}\sigma}^0(\underline{q}, \omega)$ , we have, for  $T=0$  (considered henceforth)

$$\begin{aligned} \langle \hat{S}_{\underline{k}\sigma}(\underline{q}) \hat{S}_{\underline{k}'\sigma'}(-\underline{q}) \rangle_{eq} &= (n_{\underline{k}-\underline{q}/2\sigma} - n_{\underline{k}+\underline{q}/2\sigma}) \Theta(\underline{k} \cdot \underline{q}) \delta_{\underline{k}\underline{k}'} \delta_{\sigma\sigma'} \\ &- \nu(\underline{q}) \frac{\hbar V}{\pi} \int_0^{\infty} d\omega \operatorname{Im} \left( \frac{\chi_{\underline{k}\sigma}^0(\underline{q}, \omega) \chi_{\underline{k}'\sigma'}^0(\underline{q}, \omega)}{\epsilon(\underline{q}, \omega)} \right). \quad (17) \end{aligned}$$

(continued on page 6)

We now replace  $n_{\underline{k}\sigma}$  by the non-interacting single particle momentum distribution function  $n_{\underline{k}\sigma}^0$ , and use the relation (explained in Appendix B),

$$(n_{\underline{k}-\underline{q}/2\sigma}^0 - n_{\underline{k}+\underline{q}/2\sigma}^0) \Theta(\underline{k}, \underline{q}) = (1 - n_{\underline{k}+\underline{q}/2\sigma}^0) n_{\underline{k}-\underline{q}/2\sigma}^0, \quad (18')$$

in (17) and combine the result with (6) to obtain,

$$f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q}) \cong f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q})_{HF} - v(\underline{q}) \frac{\hbar v}{\pi} \int_0^{\infty} d\omega \operatorname{Im} \left( \frac{\chi_{\underline{k}\sigma}^0(\underline{q}, \omega) \chi_{\underline{k}'\sigma'}^0(\underline{q}, \omega)}{\epsilon(\underline{q}, \omega)} \right). \quad (19)$$

Here,

$$f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q})_{HF} = -\delta_{\sigma\sigma'} \delta_{\underline{k}\underline{k}'} n_{\underline{k}-\underline{q}/2\sigma}^0 n_{\underline{k}+\underline{q}/2\sigma}^0, \quad (20)$$

is the well known Hartree Fock form for the equilibrium two particle distribution function of a non-interacting free electron system [3]. The modification to this is the second term where the longitudinal dielectric function enters incorporating the dielectric screening effect. This is our main result.

### 3. DISCUSSION

We first note that the expression for  $f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q})$  obtained here, appears to be very different from the ansätze that Aravind et al<sup>2</sup> used in their numerical calculations. The two forms that were chosen were,

$$f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q}) = f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q})_{HF} + \frac{1}{N} n_{\underline{k}\sigma}^0 n_{\underline{k}'\sigma'}^0 \{S(\underline{q}) - S^{HF}(\underline{q})\}, \quad (21a)$$

and,

$$f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q}) = f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q})_{HF} + \frac{1}{2N} \{n_{\underline{k}-\underline{q}/2\sigma}^0 n_{\underline{k}'+\underline{q}/2\sigma'}^0 + n_{\underline{k}+\underline{q}/2\sigma}^0 n_{\underline{k}'-\underline{q}/2\sigma'}^0\} \{S(\underline{q}) - S^{HF}(\underline{q})\}. \quad (21b)$$

These ansätze were so chosen that they satisfied the exact requirement given by (8) for  $f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q})$ . They were also taken to be even functions of  $\underline{q}$ .

In general, as stated earlier in (7), this assumption that,

$$f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(-\underline{q}) = f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q}),$$

which has been made by earlier workers like Niklasson<sup>1</sup> and Aravind et al<sup>2</sup>, is not accurate. Expression (19) obtained by us here does satisfy the symmetry relation (7), which we believe is an important aspect. For actual numerical calculations, suitable approximations may be made in (19) to make it amenable for computations. For example, (16a) and (16b) suggest an approximation for  $\chi_{\underline{k}\sigma\underline{k}'\sigma'}(\underline{q}, \omega)$ , viz.,

$$\chi_{\underline{k}\sigma\underline{k}'\sigma'}(\underline{q}, \omega) = \delta_{\sigma\sigma'} \delta_{\underline{k}\underline{k}'} \chi_{\underline{k}\sigma}^0(\underline{q}, \omega) / \epsilon(\underline{q}, \omega),$$

which is much simpler to handle than (13).

To see exactly how the higher order terms are included in (19), it is instructive to consider (19) to first order in  $v(\underline{q})$ , i.e., without the screening due to  $\epsilon^{-1}(\underline{q}, \omega)$  in the second term. In this case, after replacing  $\epsilon$  in (19) by unity, we can rewrite the result as,

$$f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q}) = f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q})_{HF} + \frac{v(\underline{q})}{\hbar^2 v} (\eta_{\underline{k}-\underline{q}/2\sigma}^0 - \eta_{\underline{k}+\underline{q}/2\sigma}^0) (\eta_{\underline{k}'-\underline{q}/2\sigma'}^0 - \eta_{\underline{k}'+\underline{q}/2\sigma'}^0) \cdot \frac{1}{(\underline{k}-\underline{k}') \cdot \underline{q}} [\Theta(\underline{k}' \cdot \underline{q}) - \Theta(\underline{k} \cdot \underline{q})],$$

$$= f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q})_{HF} + \frac{m}{\hbar^2 v} \frac{1}{(\underline{k}-\underline{k}') \cdot \underline{q}} v(\underline{q}) \left[ (1 - \eta_{\underline{k}+\underline{q}/2\sigma}^0) \cdot \eta_{\underline{k}-\underline{q}/2\sigma}^0 \right.$$

$$\left. (\eta_{\underline{k}'-\underline{q}/2\sigma'}^0 - \eta_{\underline{k}'+\underline{q}/2\sigma'}^0) - (1 - \eta_{\underline{k}'+\underline{q}/2\sigma'}^0) \eta_{\underline{k}'-\underline{q}/2\sigma'}^0 \right] (\eta_{\underline{k}-\underline{q}/2\sigma}^0 - \eta_{\underline{k}+\underline{q}/2\sigma}^0)$$

where in going from the first step to the second, we have made use of the equality (18).

We now compare (22) with an expression for  $f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q})$  obtained by Niklasson [3], by evaluating the first few terms of its perturbation expansion, and find that, (22) essentially contains the lowest order terms evaluated in reference 3. (see eqn. (2.19) in this reference) except for an exchange term. This difference arises from the absence of exchange contribution in our mean field approximation. The screening by  $\epsilon^{-1}(\underline{q}, \omega)$  present in (19) clearly provides ways of writing down higher order terms in  $v(\underline{q})$ .

We note that, although we have worked in the mean field (RPA) like approximation, it is possible to include the local field correction factor in a straight forward manner. If one accounts for the local field effect in (13) via a multiplying factor  $(1-G)$ , where  $G$  can be static or even a fully frequency and wavevector dependent quantity, (19) is replaced by,

$$f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q}) = f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q})_{HF} - v(\underline{q}) \frac{\pi V}{\pi} \int_0^{\infty} d\omega \operatorname{Im} \left( \frac{\chi_{\underline{k}\sigma}^{\circ}(\underline{q}, \omega) \chi_{\underline{k}'\sigma'}^{\circ}(\underline{q}, \omega) [1-G(\underline{q}, \omega)]}{\epsilon(\underline{q}, \omega)} \right) \quad (13')$$

where, now,

$$\epsilon^{-1}(\underline{q}, \omega) = \frac{1 + v(\underline{q}) \cdot \chi^{\circ}(\underline{q}, \omega)}{1 - v(\underline{q}) [1 - G(\underline{q}, \omega)] \chi^{\circ}(\underline{q}, \omega)} \quad (24')$$

We would like to emphasise now that our formulation presented here is not only independent of the actual form for  $v(\underline{q})$ , the interaction between the particles of the system, but also of the spatial dimension of the homo-

ogeneous system. This implies that formulae (19) or (20) are applicable, for example, to a two dimensional electron system in an inversion layer where a rather complicated form of  $v(\underline{q})$  appears.

Finally, we note that the extension of (19) to finite temperature  $T$  is easily obtained as (using (A.9)),

$$f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q}) = f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q})_{HF}$$

$$-v(\underline{q}) \frac{\hbar V}{\pi} \int_{-\infty}^{\infty} d\omega \operatorname{Im} \left( \frac{\chi_{\underline{k}\sigma}^0(\underline{q}, \omega) \chi_{\underline{k}'\sigma'}^0(\underline{q}, \omega)}{\epsilon(\underline{q}, \omega)} \right) \frac{1}{1 - e^{-\beta \hbar \omega}} \quad (25)$$

In the classical limit (i.e.  $\hbar \rightarrow 0$ ), this gives the following formula appropriate for a classical one component plasma:

$$f_{\underline{p}\underline{p}'}^{(2)eq}(\underline{q}) = f_{\underline{p}\underline{p}'}^{(2)eq}(\underline{q})_{free}$$

$$-v(\underline{q}) \frac{V}{\pi \beta} \int_{-\infty}^{\infty} \frac{d\omega}{\omega} \operatorname{Im} \left( \frac{\chi_{\underline{p}}^0(\underline{q}, \omega) \chi_{\underline{p}'}^0(\underline{q}, \omega)}{\epsilon(\underline{q}, \omega)} \right) \quad (26)$$

where  $\underline{p}$  and  $\underline{p}'$  are the momenta replacing  $\hbar \underline{k}$  and  $\hbar \underline{k}'$ ;

$f_{\underline{p}\underline{p}'}^{(2)eq}(\underline{q})_{free}$  and  $\chi_{\underline{p}}^0(\underline{q}, \omega)$  are given by,

$$f_{\underline{p}\underline{p}'}^{(2)eq}(\underline{q})_{free} = -\delta_{\underline{p}\underline{p}'} f^0(\underline{p}) f^0(\underline{p}')$$

$$\chi_{\underline{p}}^0(\underline{q}, \omega) = \frac{\beta}{V} \frac{\left( \frac{\underline{p} \cdot \underline{q}}{m} \right) f(\underline{p})}{\omega + i\delta - (\underline{p} \cdot \underline{q})/m}$$

with  $\chi^0(\underline{q}, \omega) = \sum_{\underline{p}} \chi_{\underline{p}}^0(\underline{q}, \omega)$  and  $f^0(\underline{p})$  representing the classical one particle momentum distribution function.

In conclusion, we note that numerical calculations using the form for  $f_{\underline{k}\sigma\underline{k}'\sigma'}^{(2)eq}(\underline{q})$  derived in this paper, would be helpful in further understanding of the advantages and limitations of the approximation.

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APPENDIX A

At any finite temperature  $T$ , we can write, [4]

$$\begin{aligned} \langle \hat{S}_{\underline{k}\sigma}^{\dagger}(\underline{q}, t) \hat{S}_{\underline{k}'\sigma'}(-\underline{q}, 0) \rangle_{eq} &= \sum_{mn} Z^{-1} e^{-\beta E_m} \\ & \langle m | e^{iHt/\hbar} \hat{S}_{\underline{k}\sigma}^{\dagger}(\underline{q}) e^{-iHt/\hbar} | n \rangle \langle n | \hat{S}_{\underline{k}'\sigma'}(-\underline{q}) | m \rangle, \\ &= \sum_{mn} Z^{-1} e^{-\beta E_m} M_{\underline{k}\sigma}^{mn}(\underline{q}) M_{\underline{k}'\sigma'}^{mn*}(-\underline{q}) e^{-i\omega_{nm}t}, \end{aligned} \quad (A.1)$$

where,

$$\hbar\omega_{nm} = E_n - E_m, \quad (A.2)$$

and, 
$$M_{\underline{k}\sigma}^{mn}(\underline{q}) = \langle m | \hat{S}_{\underline{k}\sigma}^{\dagger}(\underline{q}) | n \rangle \quad (A.3)$$

From this definition itself it follows that,

$$M_{\underline{k}\sigma}^{mn}(\underline{q}) = M_{\underline{k}\sigma}^{nm*}(-\underline{q}). \quad (A.4)$$

Similar to (A.1) we have,

$$\begin{aligned} \langle \hat{S}_{\underline{k}'\sigma'}(-\underline{q}, 0) \hat{S}_{\underline{k}\sigma}(\underline{q}, t) \rangle_{eq} \\ = \sum_{mn} Z^{-1} e^{-\beta E_m} M_{\underline{k}'\sigma'}^{mn}(-\underline{q}) M_{\underline{k}\sigma}^{mn*}(-\underline{q}) e^{i\omega_{nm}t} \end{aligned} \quad (A.5)$$

Substituting (A.1) and (A.5) in definition (9) for  $\chi_{\underline{k}\sigma\underline{k}'\sigma'}(\underline{q}, \omega)$ , we obtain the temporal Fourier transform of the imaginary part of  $\chi_{\underline{k}\sigma\underline{k}'\sigma'}(\underline{q}, \omega)$  to be,

$$\begin{aligned} \text{Im } \chi_{\underline{k}\sigma\underline{k}'\sigma'}(\underline{q}, \omega) &= -\frac{\hbar}{\pi V} \sum_{mn} Z^{-1} e^{-\beta E_m} [M_{\underline{k}\sigma}^{mn}(\underline{q}) M_{\underline{k}'\sigma'}^{mn*}(\underline{q}) \delta(\omega - \omega_{nm}) \\ & \quad - M_{\underline{k}'\sigma'}^{mn}(-\underline{q}) M_{\underline{k}\sigma}^{mn*}(-\underline{q}) \delta(\omega + \omega_{nm})]. \end{aligned} \quad (A.6)$$

Due to the inversion symmetry of the system, the matrix elements are real. Using this fact and (A.4), we can write the second term in (A.6) as,

$$\begin{aligned} \sum_{mn} M_{\underline{k}'\sigma'}^{mn}(-\underline{q}) M_{\underline{k}\sigma}^{mn*}(-\underline{q}) \delta(\omega + \omega_{nm}) Z^{-1} e^{-\beta E_m} \\ = \sum_{mn} M_{\underline{k}'\sigma'}^{nm}(\underline{q}) M_{\underline{k}\sigma}^{nm}(\underline{q}) \delta(\omega + \omega_{nm}) Z^{-1} e^{-\beta E_m}, \\ = \sum_{mn} Z^{-1} e^{-\beta E_n} M_{\underline{k}'\sigma'}^{mn}(\underline{q}) M_{\underline{k}\sigma}^{mn}(\underline{q}) \delta(\omega - \omega_{mn}), \end{aligned} \quad (A.7)$$

where in going from the second line to the third, we have interchanged the summation indices using (A.7), we have,

$$\text{Im } \chi_{\underline{k}\sigma \underline{k}'\sigma'}(\underline{q}, \omega) = (1 - e^{-\beta\hbar\omega}) \left(-\frac{\pi}{\hbar V}\right) \sum_{mn} z^{-1} e^{-\beta E_m} \cdot M_{\underline{k}\sigma}^{mn}(\underline{q}) M_{\underline{k}'\sigma'}^{mn}(\underline{q}) \delta(\omega - \omega_{nm}). \quad (\text{A.8})$$

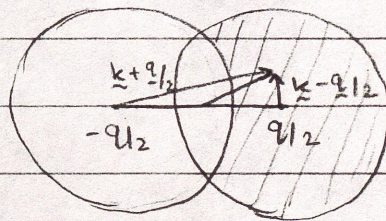
It then follows directly that,

$$\begin{aligned} \langle \hat{\xi}_{\underline{k}\sigma}(\underline{q}) \hat{\xi}_{\underline{k}'\sigma'}(-\underline{q}) \rangle_{\text{eq}} &= \sum_{mn} z^{-1} e^{-\beta E_m} M_{\underline{k}\sigma}^{mn}(\underline{q}) M_{\underline{k}'\sigma'}^{mn}(\underline{q}), \\ &= \left(-\frac{\hbar V}{\pi}\right) \int_{-\infty}^{\infty} d\omega \text{Im } \chi_{\underline{k}\sigma \underline{k}'\sigma'}(\underline{q}, \omega) \frac{1}{1 - e^{-\beta\hbar\omega}}. \quad (\text{A.9}) \end{aligned}$$

At  $T=0$ , (i.e. taking  $\beta \rightarrow \infty$  limit), the expression (A.9) reduces to (10)

### APPENDIX B.

From purely geometric considerations, it can be easily seen that, the equality given by (18) holds. In the adjoining figure we have two spheres of unit radius with centres separated by a distance  $q$ .



Since,  $n_{\underline{k}\sigma}^0 = \Theta(1 - |\underline{k}|)$ , ( $\underline{k}$  is expressed in units of  $k_F$ , the Fermi wave vector), from the figure it follows that the region where both sides of the equality (18) are non-zero and equivalent, is the shaded region in the figure.

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ON THE EQUILIBRIUM TWO PARTICLE WIGNER DISTRIBUTION FUNCTION FOR AN ELECTRON GAS

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We present here an expression for the equilibrium two particle Wigner distribution function  $f_{k\sigma k'\sigma'}^{(2)eq}(q)$ , within the mean field approximation, using the equation of motion approach. We show that the modification to the non-interacting form for  $f_{k\sigma k'\sigma'}^{(2)eq}(q)$  can be incorporated through the longitudinal dielectric function, in a manner consistent with the dielectric response theory.

1. INTRODUCTION

THE EQUILIBRIUM TWO PARTICLE Wigner distribution function  $f_{k\sigma k'\sigma'}^{(2)eq}(q)$ , is a quantity that often appears in equation of motion approaches employed to study the many body effects in the homogeneous electron gas [1]. However, an expression for this function, even in the simplest approximation, has not been made available so far. On the other hand, any theory based on the equation of motion for the two particle distribution function (e.g. calculation recently carried out by Aravind *et al.* [2]) requires, as input, the form for  $f_{k\sigma k'\sigma'}^{(2)eq}(q)$ . The aim of this paper, therefore, is to obtain an expression for  $f_{k\sigma k'\sigma'}^{(2)eq}(q)$ . For this purpose we employ the equation of motion approach and work within the mean field approximation [5].

In Section 2, we give definitions of some relevant quantities and enumerate certain general properties of the equilibrium function. In Section 3, we describe the equation of motion approach and obtain an expression for  $f_{k\sigma k'\sigma'}^{(2)eq}(q)$ . Finally in Section 4 we discuss the implications of our result.

2. DEFINITIONS AND GENERAL PROPERTIES

We begin with the definition of the non-equilibrium form for the irreducible two particle distribution function in real space, given by

$$f_{k\sigma k'\sigma'}^{(2)}(\mathbf{r}, \mathbf{r}', t) = \frac{1}{V^2} \int d^3x d^3x' e^{i\mathbf{k}\cdot\mathbf{x} + i\mathbf{k}'\cdot\mathbf{x}'} \times \left\langle \left\langle \psi_{\sigma}^+(\mathbf{r} + \frac{\mathbf{x}}{2}, t) \psi_{\sigma'}^+(\mathbf{r}' + \frac{\mathbf{x}'}{2}, t) \right. \right.$$

$$\times \left. \left. \psi_{\sigma}(\mathbf{r}' - \frac{\mathbf{x}'}{2}, t) \psi_{\sigma'}(\mathbf{r} - \frac{\mathbf{x}}{2}, t) \right\rangle \right. \\ - \left. \left. \left\langle \psi_{\sigma}^+(\mathbf{r} + \frac{\mathbf{x}}{2}, t) \psi_{\sigma'}(\mathbf{r} - \frac{\mathbf{x}}{2}, t) \right\rangle \right. \\ \times \left. \left. \left\langle \psi_{\sigma}^+(\mathbf{r}' + \frac{\mathbf{x}'}{2}, t) \psi_{\sigma'}(\mathbf{r}' - \frac{\mathbf{x}'}{2}, t) \right\rangle \right\} \quad (1)$$

where  $\psi_{\sigma}$  are the usual field operators for the interacting electrons of spin  $\sigma$  in a large volume  $V$ . In the Fourier space, it can be expressed in terms of the usual creation and annihilation operators  $a_{k\sigma}^+$  and  $a_{k\sigma}$  respectively as,

$$f_{k\sigma k'\sigma'}^{(2)}(\mathbf{q}, \mathbf{q}', t) = \langle a_{\mathbf{k}-\mathbf{q}/2\sigma}^+(t) a_{\mathbf{k}'-\mathbf{q}'/2\sigma'}^+(t) a_{\mathbf{k}'+\mathbf{q}'/2\sigma'}(t) \\ \times a_{\mathbf{k}+\mathbf{q}/2\sigma}(t) \rangle - \langle a_{\mathbf{k}-\mathbf{q}/2\sigma}^+(t) \\ \times a_{\mathbf{k}+\mathbf{q}/2\sigma}(t) \rangle \langle a_{\mathbf{k}'-\mathbf{q}'/2\sigma'}^+(t) \\ \times a_{\mathbf{k}'+\mathbf{q}'/2\sigma'}(t) \rangle. \quad (2)$$

In terms of the density fluctuation operators  $\hat{\hat{Q}}_{k\sigma}(\mathbf{q})$ , as defined as

$$\hat{\hat{Q}}_{k\sigma}(\mathbf{q}, t) = \hat{Q}_{k\sigma}(\mathbf{q}, t) - \langle \hat{Q}_{k\sigma}(\mathbf{q}, t) \rangle, \quad (3a)$$

with

$$\hat{Q}_{k\sigma}(\mathbf{q}, t) = a_{\mathbf{k}-\mathbf{q}/2\sigma}^+(t) a_{\mathbf{k}+\mathbf{q}/2\sigma}(t), \quad (3b)$$

we can rewrite (2) as

$$f_{k\sigma k'\sigma'}^{(2)}(\mathbf{q}, \mathbf{q}', t) = \langle \hat{\hat{Q}}_{k\sigma}(\mathbf{q}, t) \hat{\hat{Q}}_{k'\sigma'}(\mathbf{q}', t) \rangle \\ - \delta_{\sigma\sigma'} \delta_{\mathbf{k}, \mathbf{k}+\mathbf{q}+\mathbf{q}'} \frac{1}{2} \langle \hat{\hat{Q}}_{\mathbf{k}+\mathbf{q}/2\sigma}(\mathbf{q} + \mathbf{q}', t) \rangle. \quad (4)$$

In equilibrium, i.e., in the absence of an external field, we have

$$\langle \hat{\hat{Q}}_{k\sigma}(\mathbf{q}) \rangle_{eq} = n_{k\sigma} \delta_{\mathbf{q},0}, \quad (5)$$

where  $n_{k\sigma}$  is the single particle momentum distribution function for the interaction system. Using (5), the

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equilibrium two particle distribution function can be written in terms of density fluctuation operators as

$$f_{k\sigma k'\sigma'}^{(2)eq}(\mathbf{q}) \equiv \delta_{\mathbf{q}+\mathbf{q}',0} f_{k\sigma k'\sigma'}^{(2)}(\mathbf{q}, \mathbf{q}') = \langle \hat{\rho}_{k\sigma}(\mathbf{q}) \hat{\rho}_{k'\sigma'}(-\mathbf{q}) \rangle_{eq} - \delta_{\sigma\sigma'} \delta_{\mathbf{k}\mathbf{k}'} n_{\mathbf{k}-\mathbf{q}/2\sigma}, \quad (6)$$

where the first equality follows from the translational symmetry of the system. Due to rotational symmetry in a homogeneous system, it also follows that

$$f_{k\sigma k'\sigma'}^{(2)eq}(-\mathbf{q}) = f_{-k\sigma -k'\sigma'}^{(2)eq}(\mathbf{q}). \quad (7)$$

The sum over all momenta and spins gives an exact condition

$$\sum_{k\sigma k'\sigma'} f_{k\sigma k'\sigma'}^{(2)eq}(\mathbf{q}) = N[S(\mathbf{q}) - 1], \quad (8)$$

where  $S(\mathbf{q})$  is the usual static structure factor of the interacting electron system.

The first term on the right-hand side of (6) is related to a retarded response function, defined as

$$\chi_{k\sigma k'\sigma'}(\mathbf{q}, t) = \frac{\theta(t)}{i\hbar V} \langle [\hat{\rho}_{k\sigma}(\mathbf{q}, t), \hat{\rho}_{k'\sigma'}(-\mathbf{q}, 0)]_- \rangle_{eq}, \quad (9)$$

through the relation (derivation is straight forward [5] and follows standard textbook methods [4]),

$$\langle \hat{\rho}_{k\sigma}(\mathbf{q}) \hat{\rho}_{k'\sigma'}(-\mathbf{q}) \rangle_{eq} = -\frac{\hbar V}{\pi} \int_{-\infty}^{\infty} \frac{d\omega}{1 - e^{-\beta\hbar\omega}} \times \text{Im} \chi_{k\sigma k'\sigma'}(\mathbf{q}, \omega), \quad (10)$$

where  $\chi_{k\sigma k'\sigma'}(\mathbf{q}, \omega)$  is the temporal Fourier transform of  $\chi_{k\sigma k'\sigma'}(\mathbf{q}, t)$ . Thus the problem is reduced to obtaining an expression for the response function, which we do in the next section.

### 3. EXPRESSION FOR $f_{k\sigma k'\sigma'}^{(2)eq}(\mathbf{q})$

We use here the equation of motion approach to first obtain  $\chi_{k\sigma k'\sigma'}(\mathbf{q}, t)$ . From the definition (9), we have

$$i\hbar \frac{\partial}{\partial t} \chi_{k\sigma k'\sigma'}(\mathbf{q}, t) = \frac{\delta(t)}{V} \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} (n_{\mathbf{k}-\mathbf{q}/2\sigma} - n_{\mathbf{k}+\mathbf{q}/2\sigma}) + \frac{\theta(t)}{V} \left\langle \left[ \frac{\partial \hat{\rho}_{k\sigma}}{\partial t}(\mathbf{q}, t), \hat{\rho}_{k'\sigma'}(-\mathbf{q}, 0) \right]_- \right\rangle_{eq},$$

where we have used the commutation properties of the density fluctuation operators and (5) to write the first term. The equation of motion for  $\hat{\rho}_{k\sigma}(\mathbf{q}, t)$ , using the fully interacting Hamiltonian, is given by

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}_{k\sigma}(\mathbf{q}, t) = \frac{\hbar^2}{m} (\mathbf{k} \cdot \mathbf{q}) \hat{\rho}_{k\sigma}(\mathbf{q}, t) + \frac{1}{V} \sum_{\mathbf{q}_1 \neq 0} v(\mathbf{q}_1) \hat{\rho}(\mathbf{q}_1, t) [\hat{\rho}_{\mathbf{k}-\mathbf{q}_1/2\sigma}(\mathbf{q} - \mathbf{q}_1, t)$$

$$- \hat{\rho}_{\mathbf{k}+\mathbf{q}_1/2\sigma}(\mathbf{q} - \mathbf{q}_1, t)], \quad (12)$$

where  $v(\mathbf{q}) (= 4\pi e^2/q^2)$  is the spatial Fourier transform of the interaction between the electrons, and  $\hat{\rho} (= \sum \hat{\rho}_{k\sigma})$  is the density operator.

Substitution of (12) in (11) leads to higher order correlations entering the equation. In the present work, we restrict ourselves to the mean field (i.e. time-dependent Hartree or RPA like) approximation and hence rewrite (12) as

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}_{k\sigma}(\mathbf{q}, t) = \frac{\hbar^2}{m} (\mathbf{k} \cdot \mathbf{q}) \hat{\rho}_{k\sigma}(\mathbf{q}, t) + \frac{1}{V} v(\mathbf{q}) (n_{\mathbf{k}-\mathbf{q}/2\sigma} - n_{\mathbf{k}+\mathbf{q}/2\sigma}) \hat{\rho}(\mathbf{q}, t).$$

Substituting the above in (11) and taking its temporal Fourier transform we have

$$\chi_{k\sigma k'\sigma'}(\mathbf{q}, \omega) = \chi_{k\sigma}^0(\mathbf{q}, \omega) \times \left[ \delta_{\sigma\sigma'} \delta_{\mathbf{k}\mathbf{k}'} + \frac{v(\mathbf{q}) \chi_{k'\sigma'}^0(\mathbf{q}, \omega)}{\varepsilon(\mathbf{q}, \omega)} \right]. \quad (13)$$

Here, we have defined

$$\chi_{k\sigma}^0(\mathbf{q}, \omega) = \frac{1}{\hbar V} \frac{(n_{\mathbf{k}-\mathbf{q}/2\sigma} - n_{\mathbf{k}+\mathbf{q}/2\sigma})}{\omega + i\delta - \frac{\hbar}{m} \mathbf{k} \cdot \mathbf{q}}, \quad (14a)$$

$$\chi^0(\mathbf{q}, \omega) = \sum_{k\sigma} \chi_{k\sigma}^0(\mathbf{q}, \omega), \quad (14b)$$

and

$$\varepsilon(\mathbf{q}, \omega) = 1 - v(\mathbf{q}) \chi^0(\mathbf{q}, \omega). \quad (15)$$

By definition,  $\chi^0(\mathbf{q}, \omega)$  is the usual Lindhard function and  $\varepsilon$  has the standard RPA form for the longitudinal dielectric function [4].

Note that the following relations follow:

$$\sum_{k\sigma} \chi_{k\sigma k'\sigma'}(\mathbf{q}, \omega) = \chi_{k'\sigma'}^0(\mathbf{q}, \omega) / \varepsilon(\mathbf{q}, \omega), \quad (16a)$$

$$\sum_{k'\sigma'} \chi_{k\sigma k'\sigma'}(\mathbf{q}, \omega) = \chi_{k\sigma}^0(\mathbf{q}, \omega) / \varepsilon(\mathbf{q}, \omega), \quad (16b)$$

and

$$\sum_{k\sigma k'\sigma'} \chi_{k\sigma k'\sigma'}(\mathbf{q}, \omega) = \chi^0(\mathbf{q}, \omega) / \varepsilon(\mathbf{q}, \omega) \equiv \chi(\mathbf{q}, \omega). \quad (16c)$$

Clearly the condition (8), follows from (16), (10) and (4) with the static structure factor  $S(\mathbf{q})$  given by its RPA form.

Using (13) in (10) and explicitly writing the expression for the imaginary part of  $\chi_{k\sigma}^0(\mathbf{q}, \omega)$ , we have for  $T = 0$  (considered henceforth)

$$\langle \hat{\rho}_{k\sigma}(\mathbf{q}) \hat{\rho}_{k'\sigma'}(-\mathbf{q}) \rangle_{eq} = (n_{\mathbf{k}-\mathbf{q}/2\sigma} - n_{\mathbf{k}+\mathbf{q}/2\sigma})$$

$$\begin{aligned} & \times \theta(\mathbf{k} \cdot \mathbf{q}) \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} - v(\mathbf{q}) \frac{\hbar V}{\pi} \int_0^\infty d\omega \\ & \times \text{Im} \left[ \frac{\chi_{\mathbf{k}\sigma}^0(\mathbf{q}, \omega) \chi_{\mathbf{k}'\sigma'}^0(\mathbf{q}, \omega)}{\varepsilon(\mathbf{q}, \omega)} \right]. \end{aligned} \quad (17)$$

We now replace  $n_{\mathbf{k}\sigma}$  by the non-interacting single particle momentum distribution  $n_{\mathbf{k}\sigma}^0$ , and use the relation [5],

$$(n_{\mathbf{k}-\mathbf{q}/2\sigma}^0 - n_{\mathbf{k}+\mathbf{q}/2\sigma}^0) \theta(\mathbf{k} \cdot \mathbf{q}) = (1 - n_{\mathbf{k}+\mathbf{q}/2\sigma}^0) n_{\mathbf{k}-\mathbf{q}/2\sigma}^0, \quad (18)$$

in (17) and combine the result with (6) to obtain

$$\begin{aligned} f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}^{(2)eq}(\mathbf{q}) & \cong f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}^{(2)eq}(\mathbf{q})_{\text{HF}} - v(\mathbf{q}) \frac{\hbar V}{\pi} \int_0^\infty d\omega \\ & \times \text{Im} \left[ \frac{\chi_{\mathbf{k}\sigma}^0(\mathbf{q}, \omega) \chi_{\mathbf{k}'\sigma'}^0(\mathbf{q}, \omega)}{\varepsilon(\mathbf{q}, \omega)} \right]. \end{aligned} \quad (19)$$

Here

$$f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}^{(2)eq}(\mathbf{q})_{\text{HF}} = -\delta_{\sigma\sigma'} \delta_{\mathbf{k}\mathbf{k}'} n_{\mathbf{k}-\mathbf{q}/2\sigma}^0 n_{\mathbf{k}+\mathbf{q}/2\sigma'}^0, \quad (20)$$

is the well-known Hartree-Fock form for the equilibrium two particle distribution function of a non-interacting free electron system [3]. The modification to this is the second term where the longitudinal dielectric function enters (incorporating the dielectric screening effect). This is our main result.

#### 4. DISCUSSION

We first note that the expression for  $f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}^{(2)eq}(\mathbf{q})$  obtained here, appears to be very different from the ansatz that Aravind *et al.* [2] used in their numerical calculations. The two forms chosen were [2]

$$\begin{aligned} f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}^{(2)eq}(\mathbf{q}) & = f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}^{(2)eq}(\mathbf{q})_{\text{HF}} \\ & + \frac{1}{N} n_{\mathbf{k}\sigma}^0 n_{\mathbf{k}'\sigma'}^0 [S(\mathbf{q}) - S(\mathbf{q})_{\text{HF}}], \end{aligned} \quad (21a)$$

and

$$\begin{aligned} f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}^{(2)eq}(\mathbf{q}) & = f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}^{(2)eq}(\mathbf{q})_{\text{HF}} \\ & + \frac{1}{2N} [n_{\mathbf{k}-\mathbf{q}/2\sigma}^0 n_{\mathbf{k}'+\mathbf{q}/2\sigma'}^0 + n_{\mathbf{k}+\mathbf{q}/2\sigma}^0 n_{\mathbf{k}'-\mathbf{q}/2\sigma'}^0] \\ & \times [S(\mathbf{q}) - S(\mathbf{q})_{\text{HF}}]. \end{aligned} \quad (21b)$$

These ansatz were chosen so that they satisfied the exact requirement given by (8) for  $f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}^{(2)eq}(\mathbf{q})$ . They were also taken to be even functions of  $\mathbf{q}$ .

In general, as stated earlier in (7), the assumption

$$f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}^{(2)eq}(-\mathbf{q}) = f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}^{(2)eq}(\mathbf{q}),$$

which has been made by earlier workers like Niklasson [1] and Aravind *et al.* [2], is not accurate. Ex-

pression (19) obtained by us here does satisfy the symmetry relation (7), which, we believe, is an important aspect. For actual numerical calculations, suitable approximations may be made in (19) to make it amenable for computations. For example, (16a) and (16b) suggest an approximation for  $\chi_{\mathbf{k}\sigma\mathbf{k}'\sigma'}(\mathbf{q}, \omega)$ , viz.,

$$\chi_{\mathbf{k}\sigma\mathbf{k}'\sigma'}(\mathbf{q}, \omega) = \delta_{\sigma\sigma'} \delta_{\mathbf{k}\mathbf{k}'} \chi_{\mathbf{k}\sigma}^0(\mathbf{q}, \omega) / \varepsilon(\mathbf{q}, \omega),$$

which is much simpler to handle than (13).

To see exactly how the higher order terms are included in (19), it is instructive to consider (19) to first order in  $v(q)$ , i.e., without the screening due to  $\varepsilon^{-1}(\mathbf{q}, \omega)$  in the second term. In this case, after replacing  $\varepsilon$  in (19) by unity, we can rewrite the result as

$$\begin{aligned} f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}^{(2)eq}(\mathbf{q}) & = f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}^{(2)eq}(\mathbf{q})_{\text{HF}} + \frac{mv(\mathbf{q})}{\hbar^2 V} (n_{\mathbf{k}-\mathbf{q}/2\sigma}^0 - n_{\mathbf{k}+\mathbf{q}/2\sigma}^0) \\ & \times (n_{\mathbf{k}'-\mathbf{q}/2\sigma'}^0 - n_{\mathbf{k}'+\mathbf{q}/2\sigma'}^0) \frac{[\theta(\mathbf{k}' \cdot \mathbf{q}) - \theta(\mathbf{k} \cdot \mathbf{q})]}{(\mathbf{k} - \mathbf{k}') \cdot \mathbf{q}} \\ & = f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}^{(2)eq}(\mathbf{q})_{\text{HF}} + \frac{m}{\hbar^2 V} \frac{v(\mathbf{q})}{(\mathbf{k} - \mathbf{k}') \cdot \mathbf{q}} \\ & \times [(1 - n_{\mathbf{k}+\mathbf{q}/2\sigma}^0) n_{\mathbf{k}-\mathbf{q}/2\sigma}^0 (n_{\mathbf{k}'-\mathbf{q}/2\sigma'}^0 - n_{\mathbf{k}'+\mathbf{q}/2\sigma'}^0) \\ & - (1 - n_{\mathbf{k}'+\mathbf{q}/2\sigma'}^0) n_{\mathbf{k}'-\mathbf{q}/2\sigma'}^0 (n_{\mathbf{k}-\mathbf{q}/2\sigma}^0 - n_{\mathbf{k}+\mathbf{q}/2\sigma}^0)], \end{aligned} \quad (22)$$

where in going from the first step to the second, we have made use of the equality (18).

We now compare (22) with an expression for  $f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}^{(2)eq}(\mathbf{q})$  obtained by Niklasson [3], by evaluating the first few terms of its perturbation expansion and find that (22) essentially contains the lowest order terms evaluated in [3] (see equation (2.19) in this reference) except for an exchange term. This difference arises from the absence of exchange contribution in our mean field approximation. The screening by  $\varepsilon^{-1}(\mathbf{q}, \omega)$  present in (19) clearly provides ways of writing down higher order terms in  $v(\mathbf{q})$ .

We note that, although we have worked in the mean field (RPA) like approximation, it is possible to include the local field correction factor  $G$  in a straightforward manner. If one accounts for the local field effect in (13) via a multiplying factor  $(1 - G)$ , where  $G$  can be static or even a fully frequency and wave vector dependent quantity, (19) is replaced by

$$\begin{aligned} f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}^{(2)eq}(\mathbf{q}) & = f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}^{(2)eq}(\mathbf{q})_{\text{HF}} - v(\mathbf{q}) \frac{\hbar V}{\pi} \int_0^\infty d\omega \\ & \times \text{Im} \left[ \frac{\chi_{\mathbf{k}\sigma}^0(\mathbf{q}, \omega) \chi_{\mathbf{k}'\sigma'}^0(\mathbf{q}, \omega) [1 - G(\mathbf{q}, \omega)]}{\varepsilon(\mathbf{q}, \omega)} \right], \end{aligned} \quad (23)$$

where  $G(q, \omega)$  is the local field correction factor, and now

$$\varepsilon(\mathbf{q}, \omega)^{-1} = 1 + \frac{v(\mathbf{q})\chi^0(\mathbf{q}, \omega)}{1 - v(\mathbf{q})[1 - G(\mathbf{q}, \omega)]\chi^0(\mathbf{q}, \omega)}. \quad (24)$$

We should like to emphasize now that our formulation presented here is not only independent of the actual form of the interaction between the particles of the system, but also of the spatial dimension of the homogeneous system. This implies that formulae (19) and (23) are applicable, for example, to a two dimensional electron system in an inversion layer where a rather complicated form of  $v(\mathbf{q})$  appears.

Finally, we note that the extension of (19) to finite temperature  $T$  is easily obtained as,

$$f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}^{(2)eq}(\mathbf{q}) = f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}^{(2)eq}(\mathbf{q})_{\text{HF}} - v(\mathbf{q}) \frac{\hbar V}{\pi} \int_{-\infty}^{\infty} \frac{d\omega}{1 - e^{-\beta\hbar\omega}} \times \text{Im} \left[ \frac{\chi_{\mathbf{k}\sigma}^0(\mathbf{q}, \omega)\chi_{\mathbf{k}'\sigma'}^0(\mathbf{q}, \omega)}{\varepsilon(\mathbf{q}, \omega)} \right]. \quad (25)$$

In the classical limit (i.e.  $\hbar \rightarrow 0$ ), this gives the following formula appropriate for a classical one component plasma:

$$f_{\mathbf{p}\mathbf{p}'}^{(2)eq}(\mathbf{q}) = f_{\mathbf{p}\mathbf{p}'}^{(2)eq}(\mathbf{q})_{\text{free}} - v(\mathbf{q}) \frac{V}{\pi\beta} \int_{-\infty}^{\infty} \frac{d\omega}{\omega} \times \text{Im} \left[ \frac{\chi_{\mathbf{p}}^0(\mathbf{q}, \omega)\chi_{\mathbf{p}'}^0(\mathbf{q}, \omega)}{\varepsilon(\mathbf{q}, \omega)} \right]; \quad (26)$$

where  $\mathbf{p}$  and  $\mathbf{p}'$  are the momenta replacing  $\hbar\mathbf{k}$  and  $\hbar\mathbf{k}'$ ;  $f_{\mathbf{p}\mathbf{p}'}^{(2)eq}(\mathbf{q})_{\text{free}}$  and  $\chi_{\mathbf{p}}^0(\mathbf{q}, \omega)$  are given by

$$f_{\mathbf{p}\mathbf{p}'}^{(2)eq}(\mathbf{q})_{\text{free}} = -\delta_{\mathbf{p}\mathbf{p}'} f^0(\mathbf{p})f^0(\mathbf{p}'),$$

$$\chi_{\mathbf{p}}^0(\mathbf{q}, \omega) = \frac{\beta}{mV} \frac{(\mathbf{p} \cdot \mathbf{q})f^0(\mathbf{p})}{\omega + i\delta - (\mathbf{p} \cdot \mathbf{q})/m},$$

with  $\chi^0(\mathbf{q}, \omega) = \sum_{\mathbf{p}} \chi_{\mathbf{p}}^0(\mathbf{q}, \omega)$  and  $f^0(\mathbf{p})$  representing the classical one particle momentum distribution function.

In conclusion, we note that numerical calculations using the form for  $f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}^{(2)eq}(\mathbf{q})$  derived in this paper, would be helpful in further understanding of the advantages and limitations of the approximation.

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ON NON-EQUILIBRIUM DENSITY-DENSITY CORRELATION FUNCTION OF  
AN ELECTRON LIQUID AND DAMPING OF LONG WAVELENGTH PLASMONS

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The non-equilibrium behaviour of a homogeneous electron-liquid (jellium) with a time varying external field may be described via the linear response theory. The induced density is determined by the retarded density-density (d-d) response function  $\chi(q, \omega)$  of the system ( $q$  = Fourier wavevector,  $\omega$  = frequency). In mean field approaches, assuming that the system responds to an effective potential  $V_{\text{eff}}(q, \omega)$  (defined later) through the screened response function  $\chi_{\text{sc}}(q, \omega)$  (usually replaced by free electron response function  $\chi_0$ ), one obtains /1/

$$\chi(q, \omega) = \chi_{\text{sc}}(q, \omega) / [1 - \phi(q) \{1 - G(q, \omega)\} \chi_{\text{sc}}(q, \omega)] \quad (1)$$

where  $\phi(q) = 4\pi e^2/q^2$  and  $G$  = the so-called local field correction. In most theoretical approaches  $G$  is independent of  $\omega$  /1/ although in principle it should have a  $\omega$ -dependence determined by the non-equilibrium d-d correlation function. In this paper we present an approximate method of determining the latter and thereby  $G(q, \omega)$  and its effect on the damping of plasmons for small  $q$ .

In the presence of  $V_{\text{ext}}(\underline{R}, t)$  (external potential),  $V_{\text{eff}}(\underline{R}, t)$  to which the system responds via  $\chi_{\text{sc}}$  is /2/:

$$\nabla_{\underline{R}} \cdot V_{\text{eff}}(\underline{R}, t) = \nabla_{\underline{R}} \cdot V_{\text{H}}(\underline{R}, t) + \frac{1}{n} \int d\underline{x} \nabla \phi(\underline{R} - \underline{x}) C(x, t, \underline{R}, t), \quad (2)$$

where  $V_{\text{H}}$  is the screened time dependent Hartree potential and ( $h=1$  throughout),  $C(x, t, \underline{R}, t) = \text{Lt}(t, t) \cdot i\pi(x, t, \underline{x}, t)$  with  $i\pi(x, t, \underline{x}', t') = \langle T \{ \hat{\rho}(x, t) \hat{\rho}(\underline{x}', t') \} \rangle - \langle \hat{\rho}(x, t) \rangle \langle \hat{\rho}(\underline{x}', t') \rangle$ . Here  $\pi$  is the proper time ordered d-d correlation function of the interacting system in the presence of the external potential (i.e. in non-equilibrium) and is determined by

$$\pi(1, 1') = \pi_{\text{sc}}(1, 1') + \int \pi_{\text{sc}}(1, 2) \phi(2, 3) \pi(3, 1') d(2) d(3) \quad (3)$$

with  $\pi_{\text{sc}}$  = screened correlation function. For  $V_{\text{ext}}=0$ ,  $\pi$  reduces to  $\chi$

and  $\pi_{sc}$  to  $\chi_{sc}$ . Then:

$$\pi(1,1) = \chi(1,1) + \int \epsilon^{-1}(1,2) \bar{n}(2,3) \chi(3,1) d(2)d(3) \quad (4)$$

where  $\epsilon$  is the dielectric function and /2/

$$\bar{n}(1,1) = \int \{ \pi_{sc}(1,2) - \chi_{sc}(1,2) \} \chi_{sc}^{-1}(2,1) d(2) \quad (5)$$

The correlation functions are short ranged in space and time /2/ and therefore  $\bar{n}(1,1)$  can be approximated by  $\delta(1,1) \cdot \bar{n}(1)/n$ . Then in Fourier space,  $V_{eff}(q,w) = V_H(q,w) - \phi(q) G(q,w) n(q,w)$ ,

$$\text{where } G(q,w) = - \frac{i}{n^2} \int \frac{d^3 q' dw'}{(2\pi)^4} \frac{\bar{q} \cdot \bar{q}'}{q^2} \frac{\chi(q - q', w' - w)}{\epsilon(q', w')} \quad (6)$$

with  $\epsilon^{-1} = 1 + \phi \chi$ . This leads to expression (1). One can rewrite  $G(q,w)$  (using the definition of  $\epsilon^{-1}$  and static structure factor  $S(q)$ ) as  $G = G_1 + G_2$ , where

$$G_1 = - \frac{1}{n^2} \int \frac{d^3 q'}{(2\pi)^3} \frac{\bar{q} \cdot \bar{q}'}{q^2} [S(q' - q) - 1] \quad (7)$$

$$G_2 = - \frac{i}{n^2} \int \frac{d^3 q' dw'}{(2\pi)^4} \frac{q \cdot q'}{q^2} \phi(q') \chi(q', w') \chi(q' - q, w' - w) \quad (8)$$

The part  $G_1$  is the  $w$ -independent  $G(q)$  of Singwi et al /1/. It is real and corresponds to the high  $w$ -limit of  $G(q,w)$ . The part  $G_2$  is complex and its imaginary part determines the damping of plasmons:

$$\text{Im } G(q,w) = \frac{q}{32\pi^5} \int_0^\infty dq' \int_{-1}^{+1} dt q q' t q''^2 \int_0^\omega d\omega' Q''(q', \omega') Q''(q', \omega - \omega'), \quad (9)$$

where  $Q(q,w) = -\phi(q) \chi(q,w)$ ,  $q''^2 = q^2 + q'^2 - 2qq't$  and  $q, q'$  are in units of  $q_F$  (Fermi wavevector) and  $w, w'$  in  $\epsilon_F$  (Fermi energy).

It is gratifying to note that coupling between modes of the interacting system (e.g. particle hole pairs and plasmons) control  $G$  and in this sense our approach is parallel to the Mori formalism /3/. Here  $G_2$  should be determined self-consistently. However, we can approximate  $\chi$  by its RPA form  $\chi = \chi_0 / (1 - \phi \chi_0)$ . Thus we retain in  $G_2$  the couplings between all modes of the interacting system. Table I gives

the contributions from this coupling of modes to the damping of plasmons for small  $q$  and  $r_s=2$ . The contribution to plasmon width at  $w=w_0$  is mainly due to particle-hole part of  $Q''$ , and is considerably less than the case when  $Q''$  is approximated by  $Q''_0$ . The latter is also smaller than the Mori formulation /3/ result where too  $Q''$  is replaced by  $Q''_0$ . However in Mori formulation, the coefficient before  $Q'' Q''$  in expression (9) is different because of the difference in approach.

Table I. Plasmon width in  $\epsilon_F = \gamma q_F^2 = -(w_p/2\epsilon_F)G_2''(q, w_p)$

contributions from	Damping coefficient,	from ref.3
$Q''_0 Q''_0$	0.122163	1.339512
$Q''_{ph} C''_{ph}$	0.001466	-

In conclusion we note that it is important to evaluate the non-equilibrium d-d correlation function for obtaining  $w$ - dependent  $G$ . Our method is one scheme for this, and we are examining other schemes with improvements on the present one and will report them elsewhere.

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