Pramāṇa, Vol. 26, No. 5, May 1986, pp. 441–458. © Printed in India.

Dynamic response and frequency dependent local field correction for an electron gas system

CHAYANIKA SHAH and G MUKHOPADHYAY*

Department of Physics, Indian Institute of Technology, Powai, Bombay 400076, India
*Present address: International Centre for Theoretical Physics, P.O. Box 586, Miramare, 34100 Trieste, Italy

MS received 22 July 1985; revised 5 February 1986

Abstract. We present here an approximate scheme to obtain the complex frequency-dependent local field correction, $G(q, \omega)$. Using the equation of motion approach we develop here a methodology from which the results obtained by earlier workers, for density-density response function of an electron gas, can be arrived at in a simple systematic manner. We study in detail an approximation made along the similar lines as Singwi and coworkers, which leads to a compact expression for a complex frequency-dependent local field correction. We give results for damping coefficient of long wavelength plasmons which depends on $\mathrm{Im}\, G(q, \omega)$. The real and imaginary parts of $G(q, \omega)$ as functions of ω for various values of q are also calculated. The dynamic structure factor $S(q, \omega)$ is evaluated for $q = 1{\cdot}6\, q_F$ and compared with earlier theoretical and experimental results.

Keywords. Dynamic local field correction; density-density response function; density-density correlation function.

PACS No. 71·45

1. Introduction

The dielectric function of a uniform electron gas at metallic densities has been a quantity of interest for the past few decades mainly because of its central role in explaining metallic properties. In the past, major efforts have been made in developing a theory of the wave-vector and frequency-dependent dielectric function, with suitable approximations amenable to numerical computations. However, the numerical aspect has always set severe constraints on the nature of approximation, restricting most of the available work to approximations accurate in the long wavelength or high frequency limits. For example, the well-known time-dependent Hartree mean-field theory (also known as random phase approximation or RPA) takes proper account of only the long range part of the Coulomb interaction via screening, explaining some of the metallic properties (Singwi and Tosi 1981). However, RPA fails to describe correctly the short range part of exchange and correlation effects, for example, giving negative values of the pair correlation function $g(r)$ at short distances. Several attempts have been made in recent years to go beyond the RPA using different theoretical approaches. Most of these theories try to consider the fact that due to the short range exchange and correlation effects, there is a local depletion in the density around each electron, i.e., there exists an exchange-correlation hole around each electron. This leads to the modification of the

time-dependent Hartree mean field and one refers to the difference between the effective field and the mean field as the local field correction.

Most theories (Singwi and Tosi 1981; Singwi *et al* 1968, 1970; Vashishta and Singwi 1972; Pathak and Vashishta 1973; Toigo and Woodruff 1970, 1971) assume that this local field correction is a static and real quantity usually denoted by $G(\mathbf{q})$. The assumption of a static local field implies that each electron, under the influence of an external perturbing field, moves with its exchange and correlation hole held rigidly around it. This assumption can be true only if the perturbing force changes very slowly with time. In such a case the electrons respond almost instantaneously and the exchange correlation hole can adjust itself continuously to the motion of the electron with negligible deviation from its static value. In case the perturbing force is rapidly varying, the behaviour of the exchange-correlation hole is much more complicated. It distorts appreciably and also performs dynamic motion with respect to the electron (Holas *et al* 1979). To account for these effects, the local field correction has to be a complex, frequency-dependent quantity, $G(\mathbf{q}, \omega)$. The complex nature of the local field is necessary to include dissipative effects which lead to the damping of long wavelength plasmons. Our aim in this paper is to develop such a complex, frequency-dependent local field correction for a homogeneous electron gas.

The knowledge of a dynamic local field correction is imperative now if we are to understand the results of recent inelastic electron (Zacharias 1975) and x-ray scattering (Platzman and Eisenberger 1974) experiments, in simple metals. These experiments study the energy loss spectra and hence measure the dynamic structure factor $S(\mathbf{q}, \omega)$, over a wide range of momentum transfers. The latter, $S(\mathbf{q}, \omega)$, in turn depends on the local field correction $G(\mathbf{q}, \omega)$. Theories based on static local field correction $G(\mathbf{q})$, such as RPA (where $G(\mathbf{q}) = 0$) and other mean field theories, have failed to reproduce the experimental results for $S(\mathbf{q}, \omega)$, especially for large momentum transfers. The failure of these theories is due to the neglect of the dynamic and dissipative effects in the local field correction.

Some efforts have been made to include the dynamic effects although the theories have not been very successful. The exact high frequency behaviour of $G(\mathbf{q}, \omega)$ was obtained by Niklasson (1974) who truncated the equation of motion for a two-particle Wigner distribution function. Later Aravind *et al* (1982) used a truncation scheme equivalent to making an RPA-like approximation for the two-particle distribution function. Earlier, the same authors had carried out a low order dynamic perturbation calculation (Holas *et al* 1979) for the proper polarisability—leading to dynamic $G(\mathbf{q}, \omega)$. Along similar lines Dharmawardana (1976) wrote down a perturbation series for $G(\mathbf{q}, \omega)$ but no attempt was made to evaluate it. Brosens *et al* (1976, 1977, 1980) published a series of papers of their work, where they start with the Hartree-Fock equation of motion for one-particle distribution function and solve it by a variational method. Mukhopadhyay *et al* (1975) were able to reproduce the experimentally observed structure of $S(\mathbf{q}, \omega)$ by including the life time effects of the single-particle states (see also Niklasson *et al* 1983), but this theory violates the continuity equation. The work carried out by Awa *et al* (1981, 1982a, b) is also along similar lines and suffers from the same drawbacks. Green *et al* (1982) who included more sophisticated many-body effects also found some of the observed structure in $S(\mathbf{q}, \omega)$ but it is not clear from their treatment what the precise origin of this structure is. A few authors (Mukhopadhyay and Sjolander 1978; Jindal *et al* 1977) re-examined the problem in the

frame-work of Mori formalism but the results obtained are in disagreement with experiments.

In an earlier paper (Shah and Mukhopadhyay 1984), we have given a brief outline of our theory along with a few results for damping of long wavelength plasmons. Using the equation of motion approach we report in this paper a methodology from which the results obtained by earlier workers can be obtained in a simple, systematic manner. Section 2 gives the basic approximation made for the two-particle Wigner distribution function appearing in the equation of motion for the one-particle distribution function. In this section we also illustrate how suitable approximations lead to some earlier mean field results. In §3 we discuss in detail an approximation, made along the same lines as suggested by Singwi *et al* (1970), which leads to a frequency and wave-vector dependent local field correction. Calculations and results for damping of long wavelength plasmons and for $G(q,\omega)$ at finite q and ω are discussed in §4.

2. Theoretical formulation

We have followed the equation of motion approach in our theory. We start with the equation of motion for a one-particle Wigner distribution function. In the Fourier space, the Hamiltonian for the electron system in the presence of an external potential is given by,

$$\hat{H} = \frac{\hbar^2}{2m}\sum_{\mathbf{k}_1\sigma_1} \mathbf{k}_1^2\, a^+_{\mathbf{k}_1\sigma_1} a_{\mathbf{k}_1\sigma_1} + \frac{1}{V}\sum_{\mathbf{q}'} \phi_{\text{ext}}(-\mathbf{q}', t) \sum_{\mathbf{k}_1\sigma_1} a^+_{\mathbf{k}_1-\frac{\mathbf{q}'}{2}\sigma_1} a_{\mathbf{k}_1+\frac{\mathbf{q}'}{2}\sigma_1}$$
$$+ \frac{1}{2V}\sum_{\mathbf{q}'} v(\mathbf{q}') \sum_{\substack{\mathbf{k}_1\sigma_1\\ \mathbf{k}_2\sigma_2}} a^+_{\mathbf{k}_1-\frac{\mathbf{q}'}{2}\sigma_1} a^+_{\mathbf{k}_2+\frac{\mathbf{q}'}{2}\sigma_2} a_{\mathbf{k}_2-\frac{\mathbf{q}'}{2}\sigma_2} a_{\mathbf{k}_1+\frac{\mathbf{q}'}{2}\sigma_1}, \tag{1}$$

where $\phi_{\text{ext}}(q,t)$ is the spatial Fourier transform of a time-dependent external potential; $a_{\mathbf{k}\sigma}$ and $a^+_{\mathbf{k}\sigma}$ are the annihiliation and creation operators for the electrons and $v(q)$ represents the Coulomb potential in Fourier space ($v(q=0)=0$ to compensate for positive background in the electron gas). Using the Hamiltonian in (1), the equation of motion for the one-particle distribution function is given in Fourier space by,

$$[\hbar\omega - \frac{\hbar^2}{2m}(\mathbf{k}\cdot\mathbf{q})]\bar{f}^{(1)}_{\mathbf{k}\sigma}(\mathbf{q},\omega) = (n_{\mathbf{k}-\frac{\mathbf{q}}{2}\sigma} - n_{\mathbf{k}+\frac{\mathbf{q}}{2}\sigma})\cdot\frac{1}{V}[\phi_{\text{ext}}(\mathbf{q},\omega) + v(\mathbf{q})\bar{n}(\mathbf{q},\omega)]$$
$$+ \frac{1}{V}\sum_{\mathbf{q}'} v(\mathbf{q}') \sum_{\mathbf{k}_1\sigma_1} \{\bar{f}^{(2)}_{\mathbf{k}-\frac{\mathbf{q}'}{2}\sigma\mathbf{k}_1\sigma_1}(\mathbf{q}-\mathbf{q}', \mathbf{q}', \omega)$$
$$- \bar{f}^{(2)}_{\mathbf{k}+\frac{\mathbf{q}'}{2}\sigma\mathbf{k}_1\sigma_1}(\mathbf{q}-\mathbf{q}', \mathbf{q}', \omega)\}, \tag{2}$$

where $\bar{n}(q,\omega)$ is the induced electron density. Here, we have taken the temporal Fourier transform and retained terms to linear order in the external potential. Barred quantities in the above equation and in the remaining text denote deviation of these quantities from their respective equilibrium value (i.e. their value in the absence of the external field). $f^{(2)}$ represents the irreducible two-particle distribution function, using which we

define a function

$$C^{(2)}(\mathbf{q},\mathbf{q}',t) = \sum_{\substack{\mathbf{k}\sigma \\ \mathbf{k}'\sigma'}} f^{(2)}_{\mathbf{k}\sigma\mathbf{k}'\sigma'}(\mathbf{q},\mathbf{q}',t). \tag{3}$$

The irreducible density-density correlation function $D^{(2)}$ defined as,

$$D^{(2)}(\mathbf{q},\mathbf{q}',t) = \langle \hat{\rho}(\mathbf{q},t)\hat{\rho}(\mathbf{q}',t)\rangle, \tag{4}$$

where,

$$\hat{\rho}(\mathbf{q},t) = \hat{\rho}(\mathbf{q},t) - \langle \hat{\rho}(\mathbf{q},t)\rangle, \tag{4a}$$

is related to $C^{(2)}$ via the relation,

$$D^{(2)}(\mathbf{q},\mathbf{q}',t) = C^{(2)}(\mathbf{q},\mathbf{q}',t) + \langle \hat{\rho}(\mathbf{q}+\mathbf{q}',t)\rangle. \tag{5}$$

We note that the equilibrium values of the functions $C^{(2)}$ and $D^{(2)}$ are given by,

$$C^{(2)\mathrm{eq}}(\mathbf{q},\mathbf{q}') = \delta_{\mathbf{q}+\mathbf{q}',0}\cdot N\{S(\mathbf{q})-1\}, \tag{6a}$$

and

$$D^{(2)\mathrm{eq}}(\mathbf{q},\mathbf{q}') = \delta_{\mathbf{q}+\mathbf{q}',0} N\cdot S(\mathbf{q}), \tag{6b}$$

where N is the total number of electrons in the system.

We approximate the two-particle distribution function appearing in (2), by decoupling it into one-particle functions via the function $C^{(2)}(\mathbf{q},\mathbf{q}',t)$ (defined in (3)) as given by the expression (in real space) below,

$$f^{(2)}_{\mathbf{k}\sigma\mathbf{k}'\sigma'}(\mathbf{r},\mathbf{r}',t) \cong f^{(1)}_{\mathbf{k}\sigma}(\mathbf{r},t) f^{(1)}_{\mathbf{k}'\sigma'}(\mathbf{r}',t)\cdot\frac{1}{n^2} C^{(2)}(\mathbf{r},\mathbf{r}',t). \tag{7}$$

Here n is the constant density of electrons in the metal. This decoupling means that the electron correlation contained in $f^{(2)}$ is approximated by an average momentum and spin-independent correlation function described by $C^{(2)}$. In Fourier space, we can then write,

$$f^{(2)}_{\mathbf{k}\sigma\mathbf{k}'\sigma'}(\mathbf{q},\mathbf{q}',t) \cong \frac{1}{N^2}\sum_{\mathbf{q}_1,\mathbf{q}_2} f^{(1)}_{\mathbf{k}\sigma}(\mathbf{q}-\mathbf{q}_1,t) f^{(1)}_{\mathbf{k}'\sigma'}(\mathbf{q}'-\mathbf{q}_2,t) C^{(2)}(\mathbf{q}_1,\mathbf{q}_2,t). \tag{8}$$

This approximation preserves the continuity equation, which in the Fourier space reads,

$$i\hbar\frac{\partial}{\partial t}\sum_{\mathbf{k}\sigma} f^{(1)}_{\mathbf{k}\sigma}(\mathbf{q},t) = \frac{\hbar^2}{m}\sum_{\mathbf{k}\sigma}(\mathbf{k}\cdot\mathbf{q}) f^{(1)}_{\mathbf{k}\sigma}(\mathbf{q},t).$$

This can be easily verified by substituting (8) in (2) and then summing over $\mathbf{k}\sigma$. This is an important aspect since this cannot always be checked once an approximation is made in a theory (see Mukhopadhyay and Sjölander 1978 for discussion). On substituting (8) for $f^{(2)}$ in the equation of motion for $f^{(1)}$ and again retaining terms to linear order in

ϕ_{ext}, we have

$$\bar{n}(\mathbf{q},\omega) = \{\phi_{\text{ext}}(\mathbf{q},\omega) + v(\mathbf{q})\bar{n}(\mathbf{q},\omega)\}\chi^{r0}(\mathbf{q},\omega) + \bar{n}(\mathbf{q},\omega)\cdot\frac{1}{nV}\sum_{\mathbf{q}'} v(\mathbf{q}')\{S(\mathbf{q}-\mathbf{q}')-1\}\chi^{r0}(\mathbf{q},\mathbf{q}',\omega) + \frac{1}{nV}\sum_{\mathbf{q}'} v(\mathbf{q}')\bar{C}^{(2)}(\mathbf{q}-\mathbf{q}',\mathbf{q}',\omega)\chi^{r0}(\mathbf{q},\mathbf{q}',\omega). \tag{9}$$

In the above equation,

$$\chi^{r0}(\mathbf{q},\mathbf{q}',\omega) = \frac{1}{\hbar V}\sum_{\mathbf{k}\sigma}\frac{n_{\mathbf{k}-\frac{\mathbf{q}'}{2}\sigma} - n_{\mathbf{k}+\frac{\mathbf{q}'}{2}\sigma}}{\omega + i\delta - (\hbar/m)(\mathbf{k}\cdot\mathbf{q})}, \tag{10}$$

and $\chi^{r0}(\mathbf{q},\omega) = \chi^{r0}(\mathbf{q},\mathbf{q}',\omega)$ is the usual retarded density-density response function for the free particle (or the non-interacting electron gas) system. We have here then an expression for the induced density $\bar{n}(\mathbf{q},\omega)$ which is related to the density-density response function $\chi^{r}(\mathbf{q},\omega)$ of the fully interacting electron gas, as,

$$\bar{n}(\mathbf{q},\omega) = \chi^{r}(\mathbf{q},\omega)\phi_{\text{ext}}(\mathbf{q},\omega). \tag{11}$$

Thus by making suitable approximations for $C^{(2)}(\mathbf{q},\mathbf{q}',\omega)$ in (9), we can get $\chi^{r}(\mathbf{q},\omega)$. We now show how we can arrive at the results obtained by some of the earlier mean field theories from (9) by making suitable approximations for $\bar{C}^{(2)}(\mathbf{q},\mathbf{q}',\omega)$.

If in (9), we neglect both the second and third terms in the right side of the equation i.e., neglect $C^{(2)}$ and hence the two-particle function $\bar{f}^{(2)}$ altogether, we obtain,

$$\bar{n}(\mathbf{q},\omega) = \{\phi_{\text{ext}}(\mathbf{q},\omega) + v(\mathbf{q})\bar{n}(\mathbf{q},\omega)\}\chi^{r0}(\mathbf{q},\omega).$$

Using (11), which defines $\chi^{r}(\mathbf{q},\omega)$, we obtain,

$$\chi^{r}(\mathbf{q},\omega) = \frac{\chi^{r0}(\mathbf{q},\omega)}{1 - v(\mathbf{q})\chi^{r0}(\mathbf{q},\omega)}, \tag{12}$$

which is the well-known time-dependent Hartree approximation (Singwi and Tosi 1981) (commonly known as the random phase approximation).

As the next approximation we neglect only the third term on the right side i.e. approximate $C^{(2)}$ by its equilibrium value. In this case then we have,

$$\chi^{r}(\mathbf{q},\omega) = \frac{\chi^{r0}(\mathbf{q},\omega)}{1 - v(\mathbf{q})\{1 - G(\mathbf{q},\omega)\}\chi^{r0}(\mathbf{q},\omega)}, \tag{13}$$

where $G(\mathbf{q},\omega)$ is the so-called local field correction that is given by,

$$G(\mathbf{q},\omega) = -\frac{1}{v(\mathbf{q})\chi^{r0}(\mathbf{q},\omega)}\cdot\frac{1}{nV}\sum_{\mathbf{q}'} v(\mathbf{q}')\{S(\mathbf{q}-\mathbf{q}')-1\}\chi^{r0}(\mathbf{q},\mathbf{q}',\omega). \tag{14}$$

This is the result obtained by Hasegawa and Shimizu (1975), who followed a fully quantum mechanical approach starting with the equation of motion for a one-particle

Wigner distribution function and made an approximation for $f^{(2)}_{\mathbf{k}\sigma\mathbf{k}'\sigma'}(\mathbf{r},\mathbf{r}',t)$ as suggested by Singwi *et al* (1968). Singwi *et al* (1968) (referred to hereafter as STLS) decoupled the two-particle function via the equilibrium pair correlation function as follows:

$$f^{(2)}_{\mathbf{k}\sigma\mathbf{k}'\sigma'}(\mathbf{r},\mathbf{r}',t) \cong f^{(1)}_{\mathbf{k}\sigma}(\mathbf{r},t) f^{(1)}_{\mathbf{k}'\sigma'}(\mathbf{r}',t)\{g(\mathbf{r}-\mathbf{r}')-1\}. \tag{15}$$

Here we note that if we replace $C^{(2)}(\mathbf{r},\mathbf{r}',t)$ by its equilibrium value in (7) the present approximation for $f^{(2)}$ reduces to the one used by STLS in their calculations.

In the classical limit i.e., for $\hbar \to 0$, $\chi^{r0}(\mathbf{q},\mathbf{q}',\omega)$ is given by,

$$\chi^{r0}(\mathbf{q},\mathbf{q}',\omega) \xrightarrow{\hbar \to 0} \frac{\mathbf{q}\cdot\mathbf{q}'}{\mathbf{q}^2}\chi^{r0}(\mathbf{q},\omega). \tag{16}$$

Using this limiting value, we find that in the classical limit, (13) reduces to

$$\chi^{r}(\mathbf{q},\omega) = \frac{\chi^{r0}(\mathbf{q},\omega)}{1-v(\mathbf{q})\{1-G(\mathbf{q})\}\chi^{r0}(\mathbf{q},\omega)}, \tag{17}$$

where $G(\mathbf{q})$ which is the static local field factor is given by,

$$G(\mathbf{q}) = -\frac{1}{nV}\sum_{\mathbf{q}'}\frac{\mathbf{q}\cdot\mathbf{q}'}{\mathbf{q}'^2}\{S(\mathbf{q}-\mathbf{q}')-1\}. \tag{18}$$

This is the result obtained by STLS whose approximation for decoupling of $f^{(2)}$ in the equation of motion for $\bar{f}^{(1)}$ was rather intuitive than systematic.

Hence, we see that in the present formalism, we can obtain the earlier results (obtained using different approaches), in a more simple and methodical manner.

3. Time-dependent local field

We describe here in detail the approximation that we have used to obtain a dynamic local field correction.

First of all we note the following identity,

$$\begin{aligned}
&\sum_{\mathbf{q}'} v(\mathbf{q}')\bar{C}^{(2)}(\mathbf{q}-\mathbf{q}',\mathbf{q}',\omega)\chi^{r0}(\mathbf{q},\mathbf{q}',\omega)\\
&= \tfrac{1}{2}\sum_{\mathbf{q}'} v(\mathbf{q}')\{\bar{C}^{(2)}(\mathbf{q}-\mathbf{q}',\mathbf{q}',\omega)\chi^{r0}(\mathbf{q},\mathbf{q}',\omega)\\
&\quad + \bar{C}^{(2)}(\mathbf{q}+\mathbf{q}',-\mathbf{q}',\omega)\chi^{r0}(\mathbf{q},-\mathbf{q}',\omega)\},\\
&= \tfrac{1}{2}\sum_{\mathbf{q}'} v(\mathbf{q}')\{\bar{C}^{(2)}(\mathbf{q}-\mathbf{q}',\mathbf{q}',\omega) - \bar{C}^{(2)}(\mathbf{q}+\mathbf{q}',-\mathbf{q}',\omega)\}\chi^{r0}(\mathbf{q},\mathbf{q}',\omega),\\
&= \sum_{\mathbf{q}'} v(\mathbf{q}')\bar{D}^{(2)}((\mathbf{q}-\mathbf{q}',\mathbf{q}',\omega)\chi^{r0}(\mathbf{q},\mathbf{q}',\omega),
\end{aligned} \tag{19}$$

where we have made use of the fact that $\chi^{r0}(\mathbf{q},\mathbf{q}',\omega)$ is an odd function of $\mathbf{q}'$ and the

relation between $C^{(2)}$ and $D^{(2)}$. Thus an approximation for $\bar{D}^{(2)}$, the irreducible density-density correlation function can be used instead of $\bar{C}^{(2)}$ in (9) to get $\chi'(\mathbf{q},\omega)$.

The equal time correlation function $D^{(2)}(\mathbf{r},\mathbf{r}',t)$ is related to the time ordered function $\pi(\mathbf{r},t;\mathbf{r}',t)$, as,

$$D^{(2)}(\mathbf{r},\mathbf{r}',t) = \lim_{t'\to t} i\hbar\,\pi(\mathbf{r},t;\mathbf{r}',t') \tag{20a}$$

$$= \lim_{t'\to t}[\langle T\{\hat{\rho}(\mathbf{r},t)\hat{\rho}(\mathbf{r}',t')\}\rangle - \langle\hat{\rho}(\mathbf{r},t)\rangle\langle\hat{\rho}(\mathbf{r}',t')\rangle]. \tag{20b}$$

We obtain an expression for $D^{(2)}$ (in the presence of an external field ϕ_{ext}) using an approximate solution of an integral equation for π following the method suggested by Singwi *et al* (1970) (referred to hereafter as SSTL). We start with an integral equation for the non-equilibrium function π,

$$\pi(1,1') = \pi_{sc}(1,1') + \int \pi_{sc}(1,2)v(2,3)\pi(3,1')\,d(2)\,d(3), \tag{21}$$

where, π_{sc} is the screened correlation function; $1 \equiv (\mathbf{r}_1,t_1)$, $2 \equiv (\mathbf{r}_2,t_2)$ etc., and v as before is the Coulomb interaction. Again writing π as a sum of its equilibrium value and its deviation from equilibrium i.e., as,

$$\pi(1,1') = \pi^{eq}(1,1') + \bar{\pi}(1,1'), \tag{22}$$

we can rewrite (21). Suppressing all coordinates for brevity and using the matrix notation we have,

$$\pi^{eq} + \bar{\pi} \cong \pi_{sc}^{eq} + \bar{\pi}_{sc} + \pi_{sc}^{eq} v\,\bar{\pi} + \bar{\pi}_{sc} v\pi^{eq} + \pi_{sc}^{eq} v\pi^{eq}. \tag{23}$$

Here again since the external potential ϕ_{ext} is weak, we have retained terms only to linear order in deviations from equilibrium. π^{eq} satisfies a similar integral equation as π in (21). Making use of this we have,

$$\bar{\pi} = \varepsilon^{c\,-1}\,\bar{\pi}_{sc}(\pi_{sc}^{eq})^{-1}\,\pi^{eq}, \tag{24}$$

where we have used the definition for the causal dielectric function ε^c, i.e.,

$$\varepsilon^c = 1 - \pi_{sc}^{eq}\cdot v. \tag{25}$$

Now defining a vertex function $\bar{h}(1,1')$ as,

$$\bar{h}(1,1') = \int d(2)\,\bar{\pi}_{sc}(1,2)\,\pi_{sc}^{eq\,-1}(2,1'), \tag{26}$$

the integral equation for $\pi(1,1')$ can be written as,

$$\pi(1,1') = \pi^{eq}(1,1') + \int d(2)\,d(3)\varepsilon^{c\,-1}(1,2)\bar{h}(2,3)\,\pi^{eq}(3,1'). \tag{27}$$

We now make the ad hoc approximation for this vertex function $\bar{h}$ as suggested by SSTL. Assuming that the correlation functions are short-ranged in space and time and hence depend on the local density alone, we write,

$$\bar{h}(\mathbf{r},t;\mathbf{r}',t') \cong \delta(\mathbf{r}-\mathbf{r}')\,\delta(t-t')\cdot\frac{\bar{n}(\mathbf{r},t)}{n}. \tag{28}$$

This form ensures a static limit, for the resultant response function, equal to the static results obtained earlier by STLS. Substituting this expression for $\bar{h}(\mathbf{r}, t; \mathbf{r}', t')$ in (27), the integral equation for π within this approximation is given by,

$$\pi(\mathbf{r}, t; \mathbf{r}', t') = \pi^{eq}(\mathbf{r}, t; \mathbf{r}', t') + \frac{1}{n}\int d^3\mathbf{r}_1\, dt_1\, \varepsilon^{c^{-1}}(\mathbf{r}, t; \mathbf{r}_1, t_1)\pi^{eq}(\mathbf{r}_1, t_1; \mathbf{r}', t')\bar{n}(\mathbf{r}_1, t_1).$$

The equilibrium time-ordered correlation function is nothing but the causal density-density response function $\chi^c(\mathbf{r}, t; \mathbf{r}', t')$. Thus we have, from (20a),

$$\bar{D}^2(\mathbf{r}, \mathbf{r}', t) = \frac{i}{n}\int d\mathbf{r}''dt''\varepsilon^{c^{-1}}(\mathbf{r}-\mathbf{r}'', t-t'')\chi^c(\mathbf{r}''-\mathbf{r}', t''-t')\cdot\bar{n}(\mathbf{r}'', t''),$$

$$= \frac{1}{V^2}\sum_{\mathbf{q}_1\mathbf{q}_2}\exp(i\mathbf{q}_1\cdot\mathbf{r}+i\mathbf{q}_2\cdot\mathbf{r}')\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\exp(-i\omega t)\left[\frac{i}{n}\int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}\frac{\chi^c(\mathbf{q}_2, \omega_1-\omega)}{\varepsilon^c(\mathbf{q}_1, \omega_1)}\bar{n}(\mathbf{q}_1+\mathbf{q}_2, \omega)\right]. \tag{29}$$

Using this, the Fourier transform used in (27) is given by,

$$\bar{D}^{(2)}(\mathbf{q}-\mathbf{q}', \mathbf{q}', \omega) = \frac{i}{n}\int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}\frac{\chi^c(\mathbf{q}', \omega_1-\omega)}{\varepsilon^c(\mathbf{q}-\mathbf{q}', \omega_1)}\bar{n}(\mathbf{q}, \omega). \tag{30}$$

Within the random phase approximation (to maintain consistency), we can write,

$$\varepsilon^{c^{-1}}(\mathbf{q}, \omega) = 1 + v(\mathbf{q})\chi^c(\mathbf{q}, \omega). \tag{31}$$

Substituting in (30) we find that the expression for $\bar{D}^{(2)}(\mathbf{q}-\mathbf{q}', \mathbf{q}', \omega)$ splits into two parts as given below,

$$\bar{D}^{(2)}(\mathbf{q}-\mathbf{q}', \mathbf{q}', \omega) = \bar{n}(\mathbf{q}, \omega)\left[\frac{i}{n}\int\frac{d\omega_1}{2\pi}\chi^c(\mathbf{q}', \omega_1-\omega) + \frac{i}{n}v(\mathbf{q}-\mathbf{q}')\int\frac{d\omega_1}{2\pi}\chi^c(\mathbf{q}', \omega_1-\omega)\chi^c(\mathbf{q}-\mathbf{q}', \omega_1)\right],$$

$$= \bar{n}(\mathbf{q}, \omega)\left[S(\mathbf{q}') + v(\mathbf{q}-\mathbf{q}')\frac{i}{n}\int\frac{d\omega_1}{2\pi}\chi^c(\mathbf{q}', \omega_1-\omega)\chi^c(\mathbf{q}-\mathbf{q}', \omega_1)\right]. \tag{32}$$

Substituting this form for $\bar{D}^{(2)}(\mathbf{q}-\mathbf{q}', \mathbf{q}', \omega)$ in the third term on the right side of (9) we have,

$$\sum_{\mathbf{q}'} v(\mathbf{q}')\bar{C}^{(2)}(\mathbf{q}-\mathbf{q}', \mathbf{q}', \omega)\chi^{r0}(\mathbf{q}, \mathbf{q}', \omega)$$

$$= \sum_{\mathbf{q}'} v(\mathbf{q}')\bar{D}^{(2)}(\mathbf{q}-\mathbf{q}', \mathbf{q}', \omega)\chi^{r0}(\mathbf{q}, \mathbf{q}', \omega),$$

$$= \bar{n}(\mathbf{q}, \omega)\cdot\sum_{\mathbf{q}'} v(\mathbf{q}')\left[S(\mathbf{q}')\chi^{r0}(\mathbf{q}, \mathbf{q}', \omega)\right.$$

$$+v(\mathbf{q}-\mathbf{q}')\frac{i}{n}\int\frac{d\omega_1}{2\pi}\chi^c(\mathbf{q}',\omega_1-\omega)\chi^c(\mathbf{q}-\mathbf{q}',\omega_1)\chi^{r0}(\mathbf{q},\mathbf{q}',\omega)],$$

$$=\bar{n}(\mathbf{q},\omega)\sum_{\mathbf{q}'}v(\mathbf{q}')v(\mathbf{q}-\mathbf{q}')\frac{i}{n}\int\frac{d\omega_1}{2\pi}\chi^c(\mathbf{q}',\omega_1-\omega)$$
$$\times\chi^c(\mathbf{q}-\mathbf{q}',\omega_1)\chi^{r0}(\mathbf{q},\mathbf{q}',\omega).$$

The first term in the third line of the above equations vanishes because of the fact that $S(\mathbf{q}')\chi^{r0}(\mathbf{q},\mathbf{q}',\omega)$ is an odd function of $\mathbf{q}'$. Substituting in (9), we have,

$$\bar{n}(\mathbf{q},\omega)=\{\phi_{\text{ext}}(\mathbf{q},\omega)+v(\mathbf{q})\bar{n}(\mathbf{q},\omega)\}\chi^{r0}(\mathbf{q},\omega)$$
$$+\bar{n}(\mathbf{q},\omega)\frac{1}{nV}\sum_{\mathbf{q}'}v(\mathbf{q}')\Bigg[\{S(\mathbf{q}-\mathbf{q}')-1\}$$
$$+v(\mathbf{q}-\mathbf{q}')\cdot\frac{i}{n}\int\frac{d\omega_1}{2\pi}\chi^c(\mathbf{q}',\omega_1-\omega)\chi^c(\mathbf{q}-\mathbf{q}',\omega_1)\Bigg]\chi^{r0}(\mathbf{q},\mathbf{q}',\omega). \tag{33}$$

Then from (11) we have,

$$\chi^r(\mathbf{q},\omega)=\frac{\chi^{r0}(\mathbf{q},\omega)}{1-v(\mathbf{q})\{1-G(\mathbf{q},\omega)\}\chi^{r0}(\mathbf{q},\omega)}, \tag{34}$$

where, the local field correction $G(\mathbf{q},\omega)$ is given by,

$$G(\mathbf{q},\omega)=-\frac{1}{v(\mathbf{q})\chi^{r0}(\mathbf{q},\omega)}\cdot\frac{1}{nV}\sum_{\mathbf{q}'}v(\mathbf{q}')\Bigg[\{S(\mathbf{q}-\mathbf{q}')-1\}$$
$$+v(\mathbf{q}-\mathbf{q}')\frac{i}{n}\int\frac{d\omega_1}{2\pi}\chi^c(\mathbf{q}',\omega_1-\omega)\chi^c(\mathbf{q}-\mathbf{q}',\omega_1)\Bigg]\chi^{r0}(\mathbf{q},\mathbf{q}',\omega).$$

Since $\chi^c(\mathbf{q},\omega)$ is an even function of $\mathbf{q}$ and ω, we can rewrite the above equation to obtain,

$$G(\mathbf{q},\omega)=-\frac{1}{v(\mathbf{q})\chi^{r0}(\mathbf{q},\omega)}\cdot\frac{1}{nV}\sum_{\mathbf{q}'}v(\mathbf{q}')\Bigg[\{S(\mathbf{q}-\mathbf{q}')-1\}$$
$$+v(\mathbf{q}-\mathbf{q}')\cdot\frac{i}{n}\int\frac{d\omega_1}{2\pi}\chi^c(\mathbf{q}',\omega_1)\chi^c(\mathbf{q}-\mathbf{q}',\omega-\omega_1)\Bigg]\chi^{r0}(\mathbf{q},\mathbf{q}',\omega). \tag{35}$$

When we use Hasegawa and Shimizu's approach and use this approximation suggested by SSTL for decoupling of $\bar{f}^{(2)}$, we get a similar expression for $G(\mathbf{q},\omega)$. In this case,

$$G(\mathbf{q},\omega)=-\frac{1}{v(\mathbf{q})\chi^{r0}(\mathbf{q},\omega)}\cdot\frac{1}{nV}\sum_{\mathbf{q}'}v(\mathbf{q}')\Bigg[\{S(\mathbf{q}-\mathbf{q}')-1\}$$
$$+v(\mathbf{q}')\cdot\frac{i}{n}\int\frac{d\omega_1}{2\pi}\chi^c(\mathbf{q}',\omega_1)\chi^c(\mathbf{q}-\mathbf{q}',\omega-\omega_1)\Bigg]\chi^{r0}(\mathbf{q},\mathbf{q}',\omega). \tag{36}$$

We are not able to reproduce the result exactly mainly because of the ad hoc approximation used for $\bar{h}$. By definition, the function $D^{(2)}(\mathbf{q},\mathbf{q}',\omega)$ is symmetric with

respect to exchange of variables $\mathbf{q}$ and $\mathbf{q}'$. In this approximation we see that this does not hold (see (32)). A better and more realistic approximation should give a symmetric $D^{(2)}$.

In the classical, i.e. $\hbar \to 0$ limit, using (16) and neglecting the frequency dependence of $\varepsilon(\mathbf{q}, \omega)$ in the denominator we have,

$$G(\mathbf{q}) = -\frac{1}{nV}\sum_{\mathbf{q}'}\frac{\mathbf{q}\cdot\mathbf{q}'}{\mathbf{q}'^2}\cdot\frac{1}{\varepsilon(\mathbf{q}')}\{S(\mathbf{q}-\mathbf{q}')-1\}. \tag{37}$$

This is the result obtained by SSTL. As they neglected the frequency dependence of the dielectric function in the denominator of $G(\mathbf{q}, \omega)$, they obtained a static local field $G(\mathbf{q})$ in their approximation.

From (35) we see that the first term, a real quantity, has the same form as the local field obtained by Hasegawa and Shimizu (1975) which satisfies most of the static properties of the system. The second term is the complex, frequency-dependent part which will be of interest in our present calculations.

We consider only the classical limit of (36) for our calculations. In this limit the local field can be written as,

$$G(\mathbf{q}, \omega) = G_1(\mathbf{q}) + G_2(\mathbf{q}, \omega), \tag{38}$$

where the first term $G_1(\mathbf{q})$ is the result obtained by Singwi *et al* (1968) and is given by expression (18). The second term $G_2(\mathbf{q}, \omega)$ can be further simplified using the spectral representations for the causal functions according to which,

$$\chi^c(\mathbf{q}, \omega) = -\frac{1}{\pi}\int_0^\infty d\omega' \operatorname{Im}\chi^c(\mathbf{q}, \omega')\left\{\frac{1}{\omega-\omega'+i\delta} - \frac{1}{\omega+\omega'-i\delta}\right\}. \tag{39}$$

Using this form for the causal functions in (36) we can perform the ω_1 integral by contour integration. Then using the relation between the imaginary parts of the retarded and causal functions for positive ω (Hedin and Lundqvist 1969) the imaginary part of $G_2(\mathbf{q}, \omega)$ can be written as,

$$\operatorname{Im} G_2(\mathbf{q}, \omega) = \frac{1}{4\pi^2 e^2 n}\int\frac{d^3q'}{(2\pi)^3}\frac{\mathbf{q}\cdot\mathbf{q}'}{\mathbf{q}'^2}|\mathbf{q}-\mathbf{q}'|^2 \times \int_0^\omega d\omega_1 \, Q^{r''}(\mathbf{q}', \omega_1)\cdot Q^{r''}(|\mathbf{q}-\mathbf{q}'|, \omega-\omega_1), \tag{40}$$

where $Q^r(\mathbf{q}, \omega) = -v(\mathbf{q})\chi^r(\mathbf{q}, \omega)$, is the polarisability of the system. Using reduced units where q and q' are in units of q_F, the Fermi momentum and $\hbar\omega$ and $\hbar\omega'$ in units of ε_F, the Fermi energy, we can rewrite (40) as,

$$\operatorname{Im} G_2(q, \omega) = \frac{9}{32\alpha r_s}\int_0^\infty dq' \, q'^2 \int_{-1}^{+1} dt \, qq't \times \int_0^\omega d\omega_1 \, Q^{r''}(q', \omega_1)\cdot Q^{r''}(q'', \omega-\omega_1), \tag{41}$$

where $q''^2 = q^2 + q'^2 - 2qq't$.

In (41), the ω-dependence of $\operatorname{Im} G_2(q, \omega)$ is seen to be controlled by a product of the

type $Q^{r''}\,Q^{r''}$ i.e. by coupling between the various excitation modes of the system. A similar feature had been observed earlier by Sharma *et al* (1980) who used an entirely different approach called the Mori formalism to develop a theory mainly for investigating the damping of plasmons. In the Mori approach, a disadvantage is that the static quantities are required as inputs to the theory and cannot be extracted from the theory itself, whereas in the present case we are able to reproduce the well-accepted static results (STLS). Further, this mode coupling feature present in our approach is noteworthy because to our knowledge this is the first time, starting from an equation of motion or a generalized mean field approach, one has been able to incorporate the coupling between the excitation modes in the system.

In principle, (41) has to be solved self-consistently with (34) to obtain Im $G(q,\omega)$. The amount of computation being formidable we have replaced the Q^r in the equation for Im $G_2(q,\omega)$ by its RPA form which can be obtained from (12). By using the RPA form, we ensure the coupling between the excitation modes of the interacting system.

4. Numerical calculations and results

4.1 *Damping coefficient of long wavelength plasmons*

In the small q limit, the imaginary part of $G(\mathbf{q},\omega)$ is found to vary as q^2 (as expected). This Im $G(\mathbf{q},\omega)$ gives the plasmon damping coefficient γ which is defined (in reduced units) as,

$$\gamma = \frac{\omega_p}{2q^2}\,\mathrm{Im}\,G(q,\omega_p), \tag{42}$$

where ω_p is the bulk plasmon frequency. In table 1, we have tabulated the contributions to damping coefficient from this coupling of excitation modes for $r_s = 2$, 3, 4 and 5.

The contributions to Im $G(q,\omega)$ from interactions between particle-hole and plasmons and between plasmons themselves arise only for frequencies greater than the plasmon frequency ω_p. At $\omega \leqslant \omega_p$, the only contribution is from the $Q^{r''}_{\mathrm{ph}}\,Q^{r''}_{\mathrm{ph}}$ i.e., the particle hole part alone. When Q_{RPA} is replaced by the free electron polarisability Q^{r0}, there is a considerable increase in the value of γ. For this particular case of using non-interacting Q^{r0}, we have carried out analytical calculations also for $r_s = 2$. As q is small, we make a Taylor expansion of $Q''(\mathbf{q}'-\mathbf{q},\omega-\omega_1)$ about $\mathbf{q}'$ to linear order in $\mathbf{q}$ as,

$$Q^{r0''}(\mathbf{q}'-\mathbf{q},\omega-\omega_1) = Q^{r0''}(\mathbf{q}',\omega-\omega_1) - \mathbf{q}\cdot\nabla_{q'}Q^{r0''}(\mathbf{q}',\omega-\omega_1). \tag{43}$$

To evaluate the integrals we have followed the method suggested by Dubois (1959). In table 1 we have also listed for $r_s = 2$, the result obtained by Sharma *et al* (1980), who used Mori formalism and replaced $Q^{r''}$ by $Q^{r0''}$. The difference in the value obtained by us and that obtained by them is rather large. This is somewhat misleading because the expression obtained by Sharma *et al* (1980) viz.,

$$\gamma = \frac{3\pi}{640}\,\omega_p^3\,[63\,(1-\ln 2)] \simeq 0{\cdot}285\,\omega_p^3, \tag{44}$$

is really valid only in the $r_s \to 0$ limit. The value of γ reported in table 1 has been calculated for $r_s = 2$ using the above $r_s \to 0$ result. This small r_s result compares quite

Table 1. Contributions to damping coefficient γ calculated using equation (41) for Im $G(q, \omega_p)$.

Contributions to γ from		$r_s = 2$	$r_s = 3$	$r_s = 4$	$r_s = 5$
$Q''_{\text{RPA}} Q''_{\text{RPA}}$		0·0015	0·0023	0·0031	0·0037
$Q^{r0''} Q^{r0''}$	Computed	0·0967	0·1858	0·2293	0·3215
	Analytical	0·0966			
Result of Sharma *et al* (1980)		0·6797			

well with the weak coupling result ($r_s \to 0$) obtained earlier by Dubois and Kivelson (1969) following perturbation theory, i.e.,

$$\gamma = \frac{3\pi}{640} \omega_p^3 [34 - 22 \ln 2] \simeq 0{\cdot}276\, \omega_p^3. \tag{45}$$

We have therefore investigated the $r_s \to 0$ limit in our approximation. We use the same approximations as those used by Sharma *et al* (1980) i.e., replace $Q^{r''}$ by the free particle function $Q^{r0''}$ and neglect the second term in (43), (i.e. the derivative of Q'' $(q', \omega - \omega_1)$). In this case we obtain,

$$\gamma = \frac{3\pi}{640} \omega_p^3 [40 (1 - \ln 2)] \simeq 0{\cdot}181\, \omega_p^3. \tag{46}$$

Now the agreement with $r_s \to 0$ result of Dubois and Kivelson (1969) is fairly good and that with the result of Sharma *et al* (1980) in the same limit is far more improved. We note here that the inclusion of the derivative term in (43) reduces the value of γ by about 75%. For example, in the $r_s \to 0$ limit if we take the full expansion of $Q^{r0''}$ $(\mathbf{q} - \mathbf{q}', \omega - \omega_1)$, given in (43), we obtain,

$$\gamma = \frac{3\pi}{640} \omega_p^3 [10 (1 - \ln 2)] \simeq 0{\cdot}045\, \omega_p^3. \tag{47}$$

These results for $r_s \to 0$ however are not very useful since for metallic densities the value of r_s lies in the range between 1·8 and 5·6. Thus we feel that the γ values calculated by us and presented in table 1 are more relevant for metallic densities and none of the results (equations (44) to (47)) is meaningful in this range of r_s. However, we note that the $Q^{r0''}$ $Q^{r0''}$ approximation gives considerably large value of γ as compared with that for the more accurate fully interacting case, represented in the table by $Q''_{\text{RPA}} Q''_{\text{RPA}}$. The significant decrease in the magnitude of γ results from the screening effect which is absent in the $Q^{r0''}$ $Q^{r0''}$ approximation.

4.2 *Higher q-region*

We have calculated explicitly the Im $G_2(q,\omega)$ for various q and ω values for $r_s = 2$. In (41), Q'' is replaced by its RPA value both for particle-hole as well as plasmon part, i.e.,

$$Q^{r''} = (Q^r_{\text{RPA}})''_{\text{ph}} + (Q^r_{\text{RPA}})''_{\text{pl}}.$$

Now,

$$(Q^r_{RPA})''_{ph} = \left(\frac{Q^{r0}}{1+Q^{r0}}\right)'', \tag{48}$$

and

$$(Q^r_{RPA})''_{pl} = \frac{\pi}{2}\omega(q)\,\delta(\omega-\omega(q))\,\theta(q_c-q), \tag{49}$$

where,

$$\omega(q) = \omega_p(1+\Gamma q^2).$$

Here, $\Gamma = 9\pi/(40\alpha r_s)$ in reduced units and q_c is the critical wave vector. Thus now in $G''_2(q,\omega)$ we have contributions from $Q''_{ph}Q''_{ph}$, $Q''_{ph}Q''_{pl}$ and $Q''_{pl}Q''_{pl}$.

To obtain the particle hole contribution, we have evaluated the triple integral in (41) using numerical methods. The ω' and t integrals were evaluated together using two-dimensional Simpson's method and the value of q' integral was then calculated using trapezoidal rule. In the particle-hole plasmon part, the ω' integral could be solved

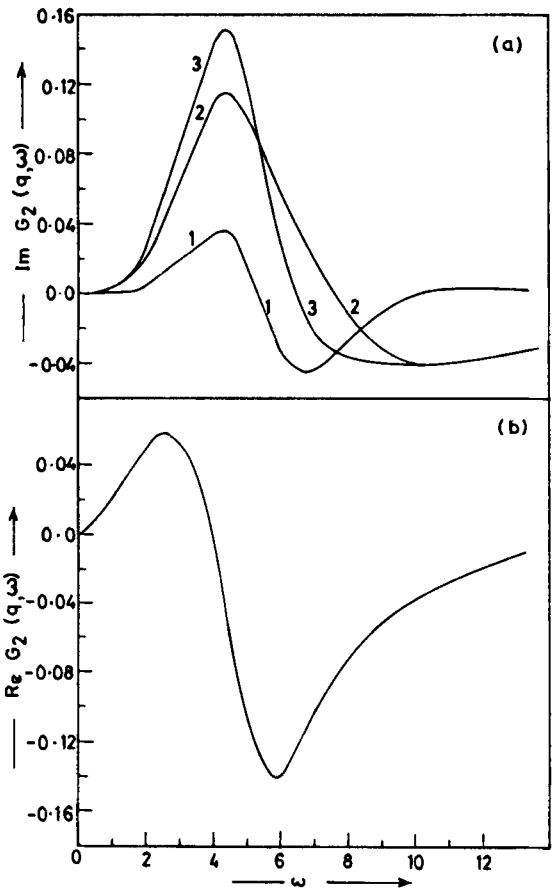

Figure 1. (a) Imaginary part of $G_2(q,\omega)$ as a function of ω for $q = 1{\cdot}6$ and $r_s = 2$. Curve 1: particle-hole plasmon part; Curve 2: particle-hole part; Curve 3: total Im $G_2(q,\omega)$. (b) Real part of $G_2(q,\omega)$ for $q = 1{\cdot}6$ and $r_s = 2$ as a function of ω.

analytically and then the t and q' integrals evaluated using numerical methods, e.g., Simpson's method for the t-integral and the trapezoidal rule method for the q' integral. The plasmon-plasmon contribution could be obtained analytically but it was found to give a non-zero value only for small q ($q < 1$ in reduced units).

In figures 1a–3a, we have plotted the different contributions to Im $G_2(q, \omega)$ and total Im $G_2(q, \omega)$, against ω for $q = 1{\cdot}6$, $2{\cdot}5$ and $5{\cdot}0$ respectively. In all these figures curve 1 gives the particle-hole plasmon part, curve 2 the particle-hole part and curve 3 the total Im $G_2(q, \omega)$. As can be seen from the curves, in the high frequency region the plasmon contribution vanishes completely and the particle-hole contribution is the only contribution. At very high ω, this $G''_{\text{ph}-\text{ph}}$ decreases to zero as $1/(A + B\omega)$.

To obtain the real part of $G_2(q, \omega)$ from this imaginary part we have made use of the Kramer-Kronig dispersion relations according to which,

$$\text{Re}\, G_2(\mathbf{q}, \omega) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\text{Im}\, G_2(\mathbf{q}, \omega')}{\omega' - \omega} \, d\omega', \tag{50}$$

where P denotes the principal value of the integral. Figures 1b–3b show the Re $G_2(q, \omega)$

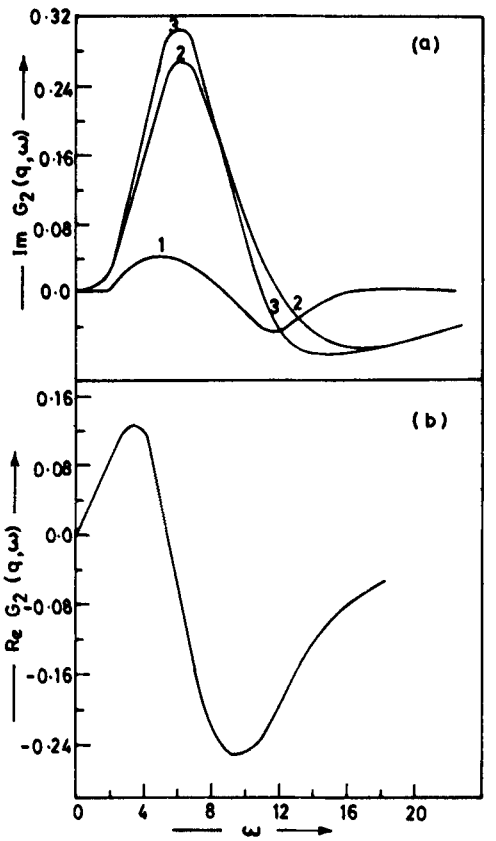

Figure 2. (**a**) Imaginary part of $G_2(q, \omega)$ as a function of ω for $q = 2{\cdot}5$ and $r_s = 2$. Curve 1: particle-hole plasmon part; Curve 2: particle-hole part; Curve 3: total Im $G_2(q, \omega)$. (**b**) Real part of $G_2(q, \omega)$ for $q = 2{\cdot}5$ and $r_s = 2$ as a function of ω.

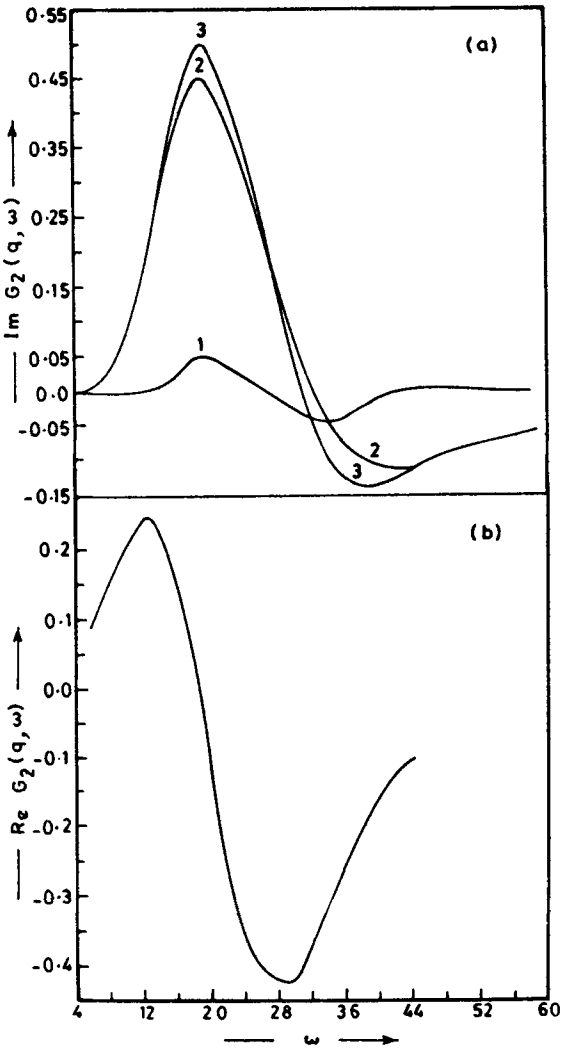

Figure 3. (a) Imaginary part of $G_2(q,\omega)$ as a function of ω for $q = 5{\cdot}0$ and $r_s = 2$. Curve 1: particle-hole plasmon part; Curve 2: particle-hole part; Curve 3: total Im $G_2(q,\omega)$. (b) Real part of $G_2(q,\omega)$ for $q = 5{\cdot}0$ and $r_s = 2$ as a function of ω.

as a function of ω, for $q = 1{\cdot}6$, $2{\cdot}5$ and $5{\cdot}0$ respectively, again for $r_s = 2$.

It is interesting to note a special feature of $G_2(q,\omega)$, viz the negative peak in its value. Niklasson (1974) had reported from his exact treatment of $G(q,\omega)$ for very large q, the existence of a strong peak at the free particle energy q^2 (in reduced units). As is seen from the curves for $G'(q,\omega)$, the peak does appear to be shifting towards the free particle energy as q increases. This is illustrated in figure 4. It should be noted that $G_2'(q,\omega)$ vanishes for both $\omega \to 0$ and $\omega \to \infty$. This means that G_2 contains the pure dynamic effects while G_1 contains the pure static effects. This is a defect in the present theory in that $G(q,\omega)$ has the same static and high frequency limits (Mukhopadhyay and Sjölander 1978, give a comparison of G at these two limits).

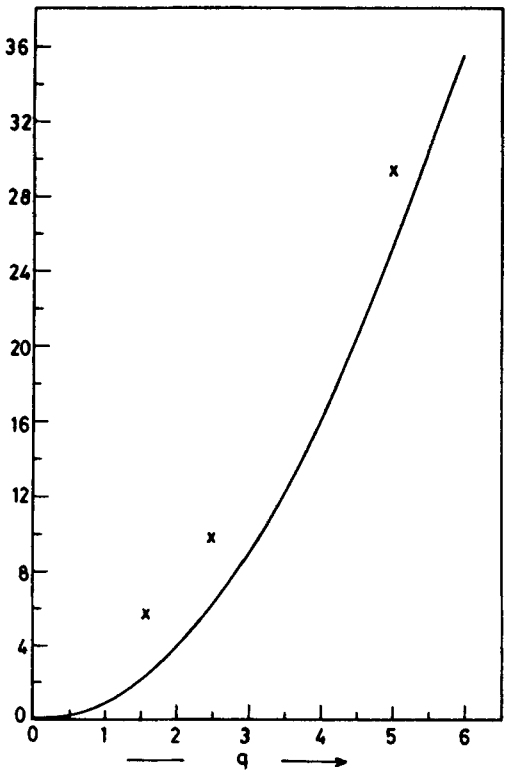

Figure 4. Solid curve is a plot for free particle energy q^2 vs q. The crosses indicate position of the negative peak in Re $G_2(q,\omega)$ for different q values. As seen from the figure, peak appears to be shifting towards free particle energy for high q.

For $q = 1{\cdot}6$, we have also calculated the dynamic structure factor $S(q,\omega)$. This quantity is related to the imaginary part of the inverse dielectric function as given by

$$\mathrm{Im}\left(\frac{1}{\varepsilon(\mathbf{q},\omega)}\right) = -\frac{4\pi^2 ne^2}{\hbar q^2} S(\mathbf{q},\omega), \tag{51}$$

and so in turn is proportional to the $Q''(q,\omega)$. To calculate the latter, we have used $G_0(q)$ in place of G_1, to obtain a better result in the static limit. In figure 5, we present our results (curve 1) for $Q''(q,\omega)$ as a function of ω for $q = 1{\cdot}6$. Curve 2 in the figure is a plot of $Q''_{\mathrm{RPA}}(q,\omega)$ and curve 3 is the experimental result (Platzman and Eisenberger 1974). All the curves have been normalized to the same peak value for comparison. As can be seen, $S(q,\omega)$ in our case has a broader peak structure than the RPA case but the peak in $S(q,\omega)$ has been shifted to a lower frequency, a trend tending towards the experimental result. The double peak structure obtained in experiments, however, is not reproduced. The calculations of Aravind *et al* (1982) also fail to show the double peak structure in $S(q,\omega)$. They have also reported a broadening in the peak as also a shift in the peak value towards lower frequency. Although Green *et al* (1982) do find some shoulder appearing in their calculations for $S(q,\omega)$, the agreement with experiment is far from good. In the present calculations for $S(q,\omega)$, a high frequency tail is also observed.

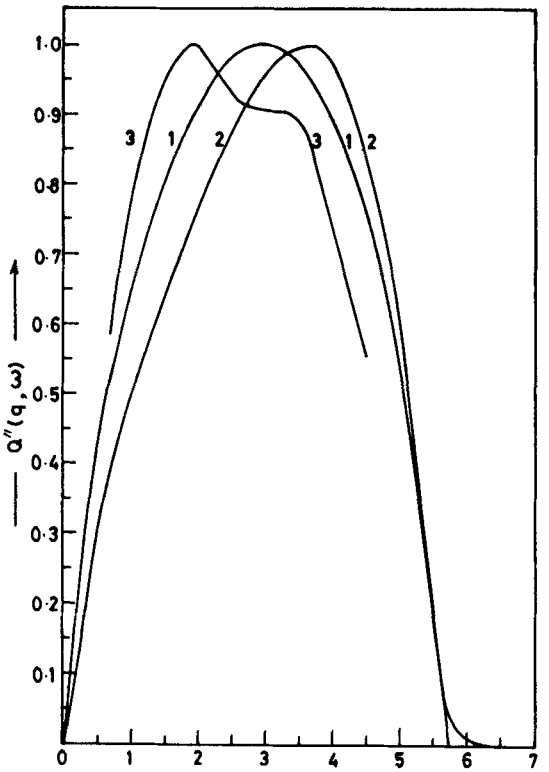

Figure 5. Plot of $Q''(q,\omega)$ vs. ω for $q = 1{\cdot}6$ and $r_s = 2$. Curve 1: Present calculations; Curve 2: RPA; Curve 3: experimental results.

5. Discussion

We have been able to develop in a systematic methodical manner, a theory that gives a complex, frequency-dependent local field correction. Also we have been able to show how suitable approximations in our theory can lead to results obtained by earlier workers in a simple, systematic manner. Further the frequency dependence in Im $G(q,\omega)$ is seen to be controlled by a term of the type $Q^{r''}\,Q^{r''}$, i.e. by coupling between excitation modes of the system. This feature had been observed earlier in an entirely different approach called the Mori formalism used for developing a mode coupling theory. To our knowledge this is the first time that such a mode coupling type term has been observed starting from an equation of motion approach. The results for damping coefficient of long wavelength plasmons at metallic densities and the fair agreement with the perturbative calculations in the weak coupling limit (Dubois and Kivelson 1969) are other positive aspects of the present theory.

A major disadvantage of the present approximation is that $G(q,\omega)$ gives the same static and high frequency limits. Also we are not able to reproduce the experimentally observed double peak structure for $S(q,\omega)$, a feature not yet explained by any of the earlier theories either. Attributing these drawbacks to the ad hoc nature of the approximation for the vertex functition $\bar{h}$, elsewhere we have developed the vertex

function in a more systematic manner, using the linear response theory (Shah 1985). The mode coupling feature is observed in that case too. Using different approaches to determine $G(q, \omega)$, we have also been able to show there, that the mode coupling feature arises due to inclusion of higher order correlations in our theory. However, from a computational point of view, the present formulation is much simpler, and gives the plasmon damping coefficient in reasonably good agreement with perturbative calculations in the weak coupling limit (Dubois and Kivelson 1969).

References

Aravind P K, Holas A and Singwi K S 1982 *Phys. Rev.* **B25** 561
Awa K, Yasuhara H and Asahi T 1981 *Solid State Commun.* **38** 1285
Awa K, Yasuhara H and Asahi T 1982a *Phys. Rev.* **B25** 3670, 3687
Brosens F, Lemmens L F and Devreese J T 1976 *Phys. Status Solidi* **B74** 45
Brosens F, Devreese J T and Lemmens L F 1977 *Phys. Status Solidi* **B80** 99
Brosens F and Lemmens L F 1980 *Phys. Rev.* **B21** 1349
Dharmawardana M W C 1976 *J. Phys.* **C9** 1919
Dubois D F 1959 *Ann. Phys.* **8** 24
Dubois D F and Kivelson M G 1969 *Phys. Rev.* **186** 409
Green F, Lowy D N and Szymánski J 1982 *Phys. Rev. Lett.* **48** 638
Hasegawa T and Shimizu M 1975 *J. Phys. Soc. Jpn* **38** 965
Hedin L and Lundqvist S 1969 *Solid State Phys.* **23** 33
Holas A, Aravind P K and Singwi K S 1979 *Phys. Rev.* **B20** 4912
Jindal V K, Singh H B and Pathak K N 1977 *Phys. Rev.* **B15** 252
Mukhopadhyay G, Kalia R K and Singwi K S 1975 *Phys. Rev. Lett.* **34** 950
Mukhopadhyay G and Sjölander A 1978 *Phys. Rev.* **B17** 3589
Niklasson G 1974 *Phys. Rev.* **B10** 3052
Niklasson G, Sjölander A and Yashida F 1983 *J. Phys. Soc. Jpn* **52** 2140
Pathak K N and Vashishta P 1973 *Phys. Rev.* **B7** 3649
Platzman P M and Eisenberger P 1974 *Phys. Rev. Lett.* **33** 152
Shah Chayanika 1985 *Many body effects in homogeneous and inhomogeneous electron systems*, Doctoral thesis submitted to I.I.T., Bombay (India), unpublished
Shah Chayanika and Mukhopadhyay G 1984 *Solid State Commun.* **52** 627
Sharma A, Monga M R and Pathak K N 1980 *Solid State Commun.* **36** 253
Singwi K S, Sjölander A, Tosi M P and Land R H 1970 *Phys. Rev.* **B1** 1044
Singwi K S and Tosi M P 1981 *Solid State Phys.* **36**
Singwi K S, Tosi M P, Land R H and Sjölander A 1968 *Phys. Rev.* **176** 589
Toigo F and Woodruff T W 1970 *Phys. Rev.* **B2** 3958
Toigo F and Woodruff T W 1971a *Phys. Rev.* **B4** 371
Toigo F and Woodruff T W 1971b *Phys. Rev.* **B4** 4312
Vashishta P and Singwi K S 1972 *Phys. Rev.* **B6** 875
Zacharias P 1975 *J. Phys.* **F5** 645