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Modified Sjölander-Stott integral equation for the electron distribution around an impurity

Bhaswati Biswas*
Cavendish Laboratory, University of Cambridge, Madingley Road, Cambridge CB3 0HE, United Kingdom
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A modification in the structure of the integral equation for the nonlinear electron distribution around a heavy impurity originally given by Sjölander and Stott has been obtained using the equation-of-motion approach for the Wigner distribution function. The modification arises due to the frequency-dependent effect in the local-field correction factor. Finally, brief remarks have been made regarding its physical significance and calculation.

I. INTRODUCTION

It is well known that nonlinear electron distributions play an important role in studies of metals. For example, the calculation of positron annihilation rates in metals requires the knowledge of a nonlinear electron distribution function. In recent years there has been an interest in the calculation of the electron density distribution around point defects such as impurities and vacancies in the electron gas. Sjölander and Stott[1] derived, sometime ago, an integral equation for the nonlinear response of electrons to the disturbance caused by a small concentration of impurities, by extending the theory of electron correlations of Singwi *et al.*[2] to the case of a two-component system consisting of electrons and impurities. Application of their theory to the problem of the charge distribution around mobile and fixed-point impurity charges gave reasonable results for negative charges. The positron annihilation rates in an electron gas for densities $r_s \leq 4$ predicted on the basis of their theory also gave good agreement with experimental values. For smaller densities $r_s \geq 5$ and the mass and charge of the positron, as also for the case of a fixed proton, the method broke down. Subsequently, Gupta, Jena, and Singwi[3,4] in a series of papers considered a modification of the nonlinear theory of Sjölander and Stott which is exact in the long-wavelength limit, and furthermore which took into account a density derivative term. In all these developments the local-field correction factor is considered to be a wave-vector-dependent real quantity usually denoted by $G(\mathbf{q})$. This assumption is justified if the perturbing field is very weak. For a varying perturbing field the local-field correction factor $G(\mathbf{q})$ is also frequency dependent and in general is a complex quantity. In this note we would like to take account of the frequency-dependent local-field correction factor $G(\mathbf{q},\omega)$ and obtain a modified integral equation for the structure factor $\gamma_{12}(\mathbf{q})$, which is the Fourier transform of the electron distribution around an impurity. The effect of the frequency-dependent local-field correction factor for a homogeneous electron gas has been studied extensively recently by Shah and Mukhopadhyay.[5,6] In our present approach we will follow the approach[6] of Shah and Mukhopadhyay and extend their results to a two-component plasma. The method is based on the equation-of-motion approach for a one-particle Wigner distribution function. The details of the method have been incorporated in Refs. 5 and 6, for the homogeneous-electron-gas problem. Similar results were also obtained by Hasegawa and Shimizu[7] starting again from the equation of motion for a one-particle Wigner distribution function. The fundamental assumption in the Singwi[3] approach to deriving the Sjölander-Stott integral equation is to write $\nabla\psi_{ij}(\mathbf{r})=g_{ij}(\mathbf{r})\nabla\phi_{ij}(\mathbf{r})$, where ψ_{ij} and ϕ_{ij} are, respectively, the effective and bare two-particle interaction and $g_{ij}(\mathbf{r})$ is the partial pair-correlation function related to $\gamma_{ij}(\mathbf{q})$ through Fourier transform. In the present method we derive systematically the relation between the effective and the bare interaction using a generalization of the equation-of-motion approach for the homogeneous electron gas. In the following section we obtain the modified integral equation for $\gamma_{12}(\mathbf{q})$ and in the final section we discuss the frequency-dependent effects on $\gamma_{12}(\mathbf{q})$.

II. MODIFICATION OF SJÖLANDER-STOTT INTEGRAL EQUATION

In this section we generalize the local-field factor to include the frequency-dependent effect in a single-impurity problem. We therefore consider a two-component plasma system consisting of electrons of density n_1 and an impurity plasma of density n_2. Following Gupta, Jena, and Singwi,[3] we write the induced density $\bar{n}_i(\mathbf{q},\omega)$ due to a weak external potential $\phi^i_{\rm ext}(\mathbf{r},t)$ acting on the ith component (here $i=1$ and 2) of the plasma system as

$$\bar{n}_i(\mathbf{q},\omega)=\sum_{j=1}^{2}\chi^r_{ij}(\mathbf{q},\omega)\phi^i_{\rm ext}(\mathbf{q},\omega)\ . \quad (1)$$

Here $\chi^r_{ij}(\mathbf{q},\omega)$ is the retarded density-density response function for the interacting system and $\phi^i_{\rm ext}(\mathbf{q},\omega)$ is the Fourier transform of the space-time-dependent external field $\phi^i_{\rm ext}(\mathbf{r},t)$. The induced density $\bar{n}_i(\mathbf{q},\omega)$ can also be written in a generalized random-phase-approximation scheme as

$$\bar{n}_i(\mathbf{q},\omega)=\chi^{r0}_i(\mathbf{q},\omega)\left[\phi^i_{\rm ext}+\sum_{j=1}^{2}\psi_{ij}(\mathbf{q},\omega)\bar{n}_j(\mathbf{q},\omega)\right]\ , \quad (2)$$

where χ^{r0}_i is the retarded density-density response function for the ith type of free particles of the system and $\psi_{ij}(\mathbf{q},\omega)$ is the effective interaction between the ith and jth components of the two-component plasma. In the equation-of-motion approach of Shah and Mukhopadhyay[6] the induced density $\bar{n}_i(\mathbf{q},\omega)$ satisfies

$$\bar{n}_i(\mathbf{q},\omega)=\chi_i^{r0}(\mathbf{q},\omega)[\phi_{\text{ext}}^i(\mathbf{q},\omega)+\phi_{ij}(\mathbf{q})\bar{n}_j(\mathbf{q},\omega)]+\frac{1}{n_1}\int\frac{d^3q'}{(2\pi)^3}\chi_i^{r0}(\mathbf{q},\mathbf{q}',\omega)\phi_{ij}(\mathbf{q}')\gamma_{ij}(\mathbf{q}-\mathbf{q}')\bar{n}_j(\mathbf{q},\omega)$$
$$+\frac{1}{n_1}\int\frac{d^3q'}{(2\pi)^3}\chi_i^{r0}(\mathbf{q},\mathbf{q}',\omega)\phi_{ij}(\mathbf{q}')\widetilde{D}_{ij}^{(2)}(\mathbf{q}-\mathbf{q}',\mathbf{q}',\omega)\bar{n}_j(\mathbf{q},\omega)\ , \tag{3}$$

where the j summation is implied and $\widetilde{D}_{ij}^{(2)}$ is related to the irreducibile density-density correlation function and is given by [see Eq. (30) of Ref. 6].

$$D_{ij}^{(2)}(\mathbf{q}-\mathbf{q},\mathbf{q}',\omega)$$
$$=\frac{i}{n_1}\int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}\chi_{ij}^c(\mathbf{q}',\omega_1-\omega)/\epsilon_{ij}^c(\mathbf{q}-\mathbf{q}',\omega_1)\ . \tag{4}$$

Here in (4), χ_{ij}^c is the causal density-density response function and in the random-phase approximation is related to the causal dielectric tensor ϵ_{ij}^c by

$$\frac{1}{\epsilon_{ij}^c(\mathbf{q},\omega)}=\delta_{ij}+\phi_{ij}\chi_{ij}^c(\mathbf{q},\omega)\ . \tag{5}$$

Comparing Eqs. (3) and (2) we easily see that in the equation-of-motion approach $\psi_{ij}(\mathbf{q},\omega)$ is given by

$$\psi_{ij}(\mathbf{q},\omega)=\phi_{ij}[1-G_{ij}^{(1)}(\mathbf{q},\omega)-G_{ij}^{(2)}(\mathbf{q},\omega)]\ , \tag{6}$$

where

$$G_{ij}^{(1)}(\mathbf{q},\omega)=-\frac{1}{n_1}\frac{1}{\phi_{ij}(\mathbf{q})}\int\frac{d^3q'}{(2\pi)^3}\frac{\chi_i^{r0}(\mathbf{q},\mathbf{q}'\omega)}{\chi_i^{r0}(\mathbf{q},\omega)}\phi_{ij}(\mathbf{q}')\times\gamma_{ij}(\mathbf{q}-\mathbf{q}') \tag{7}$$

and

$$G_{ij}^{(2)}(\mathbf{q},\omega)=-\frac{1}{n_1}\frac{1}{\phi_{ij}(\mathbf{q})}\int\frac{d^3q'}{(2\pi)^3}\frac{\chi_i^{r0}(\mathbf{q},\mathbf{q}',\omega)}{\chi_i^{r0}(\mathbf{q},\omega)}\phi_{ij}(\mathbf{q}')\times\widetilde{D}_{ij}^{(2)}(\mathbf{q}-\mathbf{q}',\mathbf{q}',\omega)\ . \tag{8}$$

The appearance of $G_{ij}^{(2)}(\mathbf{q},\omega)$ in Eq. (6) is the new addition which does not occur in the approach of Gupta *et al.*[3] In Eqs. (3), (7), and (8), $\chi_i^{r0}(\mathbf{q},\mathbf{q}',\omega)$ stands for

$$\chi_i^{r0}(\mathbf{q},\mathbf{q}',\omega)=\frac{1}{\hbar V}\sum_{\mathbf{k}}\left[\frac{n_i(\mathbf{k}-\mathbf{q}'/2)-n_i(\mathbf{k}+\mathbf{q}'/2)}{\omega-(\hbar/m_i)(\mathbf{k}\cdot\mathbf{q})+i\delta}\right]\ , \tag{9}$$

where m_i is the mass of the ith component of the plasma and further $\chi_i^{r0}(\mathbf{q},\omega)=\chi_i^{r0}(\mathbf{q},\mathbf{q},\omega)$ and V is the volume of the system. In the classical limit, i.e., for $\hbar\to 0$, we have

$$\chi_i^{r0}(\mathbf{q},\mathbf{q}',\omega)=\frac{\mathbf{q}\cdot\mathbf{q}'}{q^2}\chi_i^{r0}(\mathbf{q},\omega)\ . \tag{10}$$

We now easily see that if we drop $G_{ij}^{(2)}$ in the expression of $\psi_{ij}(\mathbf{q},\omega)$ given by Eq. (6) and utilize Eq. (10), then we recover the standard expression for ψ_{ij} as given in Refs. 1 and 3, namely,

$$\psi_{ij}=\phi_{ij}(1-G_{ij}^{(1)})$$

with

$$G_{ij}^{(1)}=-\frac{1}{n_1\phi_{ij}(\mathbf{q})}\int\frac{d^3q'}{(2\pi)^3}\frac{\mathbf{q}\cdot\mathbf{q}'}{q^2}\phi_{ij}(\mathbf{q}')\gamma_{ij}(\mathbf{q}-\mathbf{q}')\ , \tag{11}$$

which is Eq. (8) of Ref. 3.

Using Eqs. (10), (5), and (4) and the fact that $\gamma_{ij}(\mathbf{q}')\chi_i^{r0}(\mathbf{q},\mathbf{q}',\omega)$ is an odd function of q', we can also put Eq. (8), as in Ref. 6, in the following form:

$$(G_{ij}^{(2)}(\mathbf{q},\omega)=-\frac{1}{n_1\phi_{ij}(\mathbf{q})}\int\frac{d^3q'}{(2\pi)^3}\frac{\mathbf{q}\cdot\mathbf{q}'}{q^2}\phi_{ij}(\mathbf{q}')\phi_{ij}(\mathbf{q}-\mathbf{q}')\times\frac{i}{n_1}\int\frac{d\omega_1}{2\pi}\chi_{ij}^c(\mathbf{q}',\omega_1-\omega)\times\chi_{ij}^c(\mathbf{q}-\mathbf{q}',\omega_1)\ . \tag{12}$$

In the rest of our consideration we will take Eqs. (11) and (12) for $G_{ij}^{(1)}$ and $G_{ij}^{(2)}$, respectively. It results from a generalization to a two-component system of the work of Shah and Mukhopadhyay[6] on the uniform gas. The approximation scheme used by Shah and Mukhopadhyay[6] is originally due to Singwi *et al.*[8] In the limit of small impurity concentration we have from (1) and (2) the following expression for $\chi_{12}^r(\mathbf{q},\omega)$:

$$\chi_{12}^r(\mathbf{q},\omega)=\chi_{11}^r(\mathbf{q},\omega)\chi_2^{r0}(\mathbf{q},\omega)\psi_{12}(\mathbf{q},\omega)\ . \tag{13}$$

In writing down Eq. (13) we used $\chi_{12}^r=\chi_{21}^r$ and $\psi_{21}=\psi_{12}$. We now define the appropriate dielectric tensor $\epsilon_{ij}^r(\mathbf{q},\omega)$ through the retarded response function

$$\frac{1}{\epsilon_{ij}^r(\mathbf{q},\omega)}=\delta_{ij}+\phi_{ij}(\mathbf{q})\chi_{ij}^r(\mathbf{q},\omega) \tag{14}$$

and use the following relation,

$$n_i\left[\delta_{ij}+\frac{n_i}{n_1}\gamma_{ij}(\mathbf{q})\right]=-\frac{\hbar}{\pi\phi_{ij}}\int_0^{\infty}d\omega\,\mathrm{Im}\left[\frac{1}{\epsilon_{ij}^r(\mathbf{q}\cdot\omega)}\right]\ , \tag{15}$$

to obtain the modified integral equation for $\gamma_{ij}(\mathbf{q})$. Combining Eqs. (13), (14), and (15), we obtain

$$\gamma_{12}(\mathbf{q})=-\frac{\hbar}{\pi}\frac{1}{n_2}\frac{\phi_{12}}{\phi_{11}}\int_0^{\infty}d\omega\,\mathrm{Im}\left[\chi_2^{r0}(\mathbf{q},\omega)\left[\frac{1}{\epsilon_{11}^r(\mathbf{q},\omega)}-1\right]\right][1-G_{12}^{(1)}(\mathbf{q})]$$
$$+\frac{\hbar}{\pi}\frac{\phi_{12}}{n_2\phi_{11}}\int_0^{\infty}d\omega\,\mathrm{Im}\left[\chi_2^{r0}(\mathbf{q},\omega)\left[\frac{1}{\epsilon_{11}^r(\mathbf{q},\omega)}-1\right]G_{12}^{(2)}(\mathbf{q},\omega)\right]\ . \tag{16}$$

If we now use Eq. (9) then for fixed impurity n_2, we have

$$\chi_2^{r0}(\mathbf{q},\omega)=\frac{n_2}{\hbar}\left[\frac{1}{\omega-\frac{\hbar q^2}{2m_2}+i\delta}-\frac{1}{\omega+\frac{\hbar q^2}{2m_2}+i\delta}\right], \tag{17}$$

then the first integral in Eq. (16) can be easily worked out and for $m_2\to\infty$ we have for $\gamma_{12}(\mathbf{q})$ the following integral equation:

$$\gamma_{12}(\mathbf{q})=I(\mathbf{q})+\left[\frac{1}{\epsilon_{11}^r(\mathbf{q},0)}-1\right]\frac{\phi_{12}}{\phi_{11}}\left[1+\frac{1}{n_1\phi_{12}}\int\frac{d^3q'}{(2\pi)^3}\frac{\mathbf{q}\cdot\mathbf{q}'}{q^2}\phi_{12}(\mathbf{q}')\gamma_{12}(\mathbf{q}-\mathbf{q}')\right]. \tag{18}$$

Equation (18) differs from the standard Sjölander-Stott integral equation by the presence of an additional inhomogeneous term $I(\mathbf{q})$, where

$$I(\mathbf{q})=\frac{\hbar}{\pi}\frac{\phi_{12}}{n_2\phi_{11}}\int_0^\infty d\omega\,\mathrm{Im}\left[\chi_2^{r0}(\mathbf{q},\omega)\left[\frac{1}{\epsilon_{11}^r(\mathbf{q},\omega)}-1\right]G_{12}^{(2)}(\mathbf{q},\omega)\right].$$

Equation (18) is the new result of the present note. In the following section we briefly remark about the calculation of $I(\mathbf{q})$.

III. CONCLUDING REMARKS

The inhomogeneous term $I(\mathbf{q})$ given below Eq. (18) can be integrated. Since[6] $\mathrm{Im}G_{12}^{(2)}(\mathbf{q},\hbar q^2/2m_2)\to 0$ in the limit $m_2\to\infty$ (i.e., for fixed heavy impurity mass) we are left with the following expression for $I(\mathbf{q})$, namely:

$$I(\mathbf{q})=-\left[\frac{1}{\epsilon_{11}^r(\mathbf{q},0)}-1\right]\frac{\phi_{12}}{\phi_{11}}\mathrm{Re}G_{12}^{(2)}(\mathbf{q},0). \tag{19}$$

To obtain the real part of $G_{12}^{(2)}(\mathbf{q},\omega)$ when $\omega\to 0$ we use the dispersion relation

$$\mathrm{Re}G_{12}^{(2)}(\mathbf{q},0)=\frac{P}{\pi}\int_{-\infty}^{\infty}\frac{d\omega}{\omega}\mathrm{Im}G_{12}^{(2)}(\mathbf{q},\omega). \tag{20}$$

The imaginary part of $G_{12}^{(2)}(\mathbf{q},\omega)$ can be obtained from polarizability of the system due to the field ϕ_{12}. For example, from Eq. (12) one can easily calculate the imaginary part of $G_{12}^{(2)}(\mathbf{q},\omega)$ as

$$\mathrm{Im}G_{12}^{(2)}(\mathbf{q},\omega)=\frac{1}{\phi_{12}(\mathbf{q})n_1^2}\int d^3q'\frac{\mathbf{q}\cdot\mathbf{q}'}{q^2}\int_0^\omega d\omega''\,\mathrm{Im}Q^r(\mathbf{q}',\omega'')\mathrm{Im}Q^r(|\mathbf{q}-\mathbf{q}'|,\omega-\omega''), \tag{21}$$

where $Q^r(\mathbf{q},\omega)=-\phi_{12}(\mathbf{q})\chi^r(\mathbf{q},\omega)$ is the polarizability of the system. In deriving Eq. (21) we have used in Eq. (12) the dispersion relation for the causal density-density response functions $\chi_{ij}^c(\mathbf{q},\omega)$ namely,

$$\chi_{ij}^c(\mathbf{q},\omega)=\frac{-1}{\pi}\int_0^\infty d\omega'\,\mathrm{Im}\chi_{ij}^c(\mathbf{q},\omega')\times\left[\frac{1}{\omega-\omega'+i\delta}-\frac{1}{\omega+\omega'-i\delta}\right] \tag{22}$$

and the relation between the imaginary parts of retarded and causal functions for positive frequencies.[9] We thus see that a knowledge of the field $\phi_{12}(\mathbf{q})$ and the dielectric function will enable us to evaluate $\mathrm{Im}G_{12}^{(2)}(\mathbf{q},\omega)$ for practical purposes. $\mathrm{Im}G^{(2)}(\mathbf{q},\omega)$ for the case of Coulomb field has been the subject of calculation by many authors.[10] It gives the plasma damping coefficient γ defined by $\gamma=(\omega_p/2q^2)\mathrm{Im}G^{(2)}(\mathbf{q},\omega_p)$ where ω_p is the bulk plasma frequency.

Writing $\mathrm{Re}G_{12}^{(2)}(\mathbf{q},0)=G_{12}^{(2)}(\mathbf{q})$, our final equation takes the form

$$\gamma_{12}(\mathbf{q})=\left[\frac{1}{\epsilon_{11}^r(\mathbf{q},0)}-1\right]\frac{\phi_{12}(\mathbf{q})}{\phi_{11}(\mathbf{q})}\left[1-G_{12}^{(2)}(\mathbf{q})+\frac{1}{n_1\phi_{12}}\int\frac{d^3q'}{(2\pi)^3}\phi_{12}(\mathbf{q}')\gamma_{12}(\mathbf{q}-\mathbf{q}')\right]. \tag{23}$$

Equation (23) can be easily modified to incorporate the density derivative term of $\gamma_{12}(\mathbf{q})$ in the same manner as in Ref. (3).

The effect of $G_{ij}^{(2)}$ which occurs in $I(\mathbf{q})$ has altered the original Sjölander-Stott integral equation in an essential way and we hope to observe the effects in problems like the calculation of electron density distribution around impurities and positron annihilation rate in electron systems. We will report on the modification in the physical problems due to Eq. (23) in the near future.

*Permanent address: Department of Physics & Astrophysics, University of Delhi, Delhi-110007 India.

[1]A. Sjölander and M. J. Stott, Phys. Rev. B **5**, 2109 (1972).
[2]K. S. Singwi, M. P. Tosi, R. H. Land, and A. Sjölander, Phys. Rev. **176**, 589 (1968).
[3]A. K. Gupta, P. Jena, and K. S. Singwi, Phys. Rev. B **18**, 2712 (1978).
[4]P. Jena, A. K. Gupta, and K. S. Singwi, Phys. Rev. B **18**, 2723 (1978).
[5]C. Shah and G. Mukhopadhyay, Solid State Commun. **52**, 627 (1984).
[6]C. Shah and G. Mukhopadhyay, Pramana **26**, 441 (1986).
[7]T. Hasegawa and M. Shimizu, J. Phys. Soc. Jpn. **38**, 965 (1975).
[8]K. S. Singwi, A. Sjölander, M. P. Tosi, and R. H. Land, Phys. Rev. B **1**, 1044 (1970).
[9]L. Hedin and S. Lundqvist, Solid State Phys. **23**, 33 (1969).
[10]See Ref. 6 and A. Sharma *et al.*, Solid State Commun. **36**, 253 (1980).