Exchange and correlation effects in anisotropic systems

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Exchange and correlation effects in an electron gas with an anisotropic effective-mass ratio are investigated, within a self-consistent procedure beyond the random-phase approximation (RPA). The plasmon dispersion relation and the pair-correlation function are shown as a function of the electron density, mass ratio, and for selected angles of propagation. We have found sizable differences from the RPA results.

I. INTRODUCTION

Many materials, such as polymeric polysulfurnitride, $(SN)_x$, show a strong anisotropy causing their electronic properties to vary quite noticeably, according to the direction examined.[1] These materials can, in general, be understood as consisting of bundles of fibers, composed of parallel segregated chains of molecules, in which the electrons are free to move. The electronic properties of these materials are quite anisotropic due both to the microscopic structure leading to higher conductivity along the polymer chains and to the arrangement into fibers. The quasi-one-dimensional feature occurs since there is little overlap between the electronic wave functions on different chains. The interchain interactions are weak, but cannot be ignored in trying to explain some of their properties. Some of these materials have been shown to be superconducting at temperatures of the order of tenths of degree. It has been suggested that the small diameter of the fibers may lead to quasi-one-dimensional superconductivity in the temperature regime where the coherence length is large as compared with the fiber diameter.[2]

The purpose of this work is to investigate the electronic properties of anisotropic materials, within the self-consistent-field approximation, as introduced many years ago by Singwi *et al.*,[3] for the isotropic electron gas. In this method, the short-range correlation effects are taken into account through a local-field correction. The results will be shown as a function of the angle with the strand direction, the masses perpendicular and parallel to this direction, and the electron density of the system.

II. THEORETICAL FORMULATION

The self-consistent-field approximation proposed by Singwi *et al.* (hereafter referred to as STLS) has been applied for different systems leading to better results than the random-phase approximation (RPA). The RPA results are obtained from STLS simply by disregarding the local-field corrections, corresponding then to the zeroth-order interaction in STLS.[4]

Let us first introduce the effective masses $m_\parallel$ and $m_\perp$, respectively the masses parallel and perpendicular to the strand axis.[5] By choosing z as the direction of this axis, we may perform a scale transformation[6] getting an anisotropic vector $\boldsymbol{\xi}$ which plays the role of the wave vector in the anisotropic system, with components $q_x(m_\perp)^{-1/2}$, $q_y(m_\perp)^{-1/2}$, $q_z(m_\parallel)^{-1/2}$, or $\xi=q\beta(\theta)/(m_\parallel)^{-1/2}$, where $\beta(\theta)=[\cos^2\theta+\sin^2\theta/R]^{1/2}$, θ being the angle between $\mathbf{q}$ and the z axis and $R=m_\perp/m_\parallel$, the mass ratio. With this definition, the kinetic energy of a charge carrier of momentum $\hbar\mathbf{q}$ is $E(\xi)=\hbar^2\xi^2/2$. The dielectric function of the system in the STLS scheme, for the present problem, can be written as

$$\epsilon(\xi,\omega)=1+\frac{Q_0(\xi,\omega)}{1-G(\xi)Q_0(\xi,\omega)}\,, \tag{1}$$

where $Q_0(\xi,\omega)=-\phi(\xi)\chi_0(\xi,\omega)$, $\phi(\xi)=\omega_{\rm pl}^2(\theta)/\rho\xi^2$ is the bare particle-particle interaction, with the anisotropic plasma frequency $\omega_{\rm pl}(\theta)=\omega_{\rm pl}^0\beta(\theta)$ defined through the usual isotropic plasma frequency $\omega_{\rm pl}^0=(4\pi\rho e^2/m\epsilon_\infty)^{1/2}$ and the electronic density ρ.

For an anisotropic noninteracting electron system, the real and imaginary parts of the density-density response function, $\chi_0(\xi,\omega)$, are given, respectively, by

$$\mathrm{Re}\chi_0(\xi,\omega)=\frac{3\rho}{4E_F}\left[1+\left(\frac{E_F}{\lambda^3}\right)\times\left((\lambda^2-\Omega_+^2)\ln\left|\frac{\lambda+\Omega_+}{\lambda-\Omega_+}\right|-(\lambda^2-\Omega_-^2)\ln\left|\frac{\lambda+\Omega_-}{\lambda-\Omega_-}\right|\right)\right]\,, \tag{2}$$

and

$$\mathrm{Im}\chi_0(\xi,\omega)=-\frac{3\pi\rho}{4\lambda^3}[(\lambda^2-\Omega_-^2)\Phi(\lambda-|\Omega_-|)-(\lambda^2-\Omega_+^2)\Phi(\lambda-|\Omega_+|)]\,, \tag{3}$$

where $\Omega_{\pm} = \hbar\omega \pm E(\xi)$, $\lambda = 2\sqrt{E(\xi)E_F}$, and the Fermi energy $E_F = (2\hbar^2/m_\parallel)(3\pi^2\rho/R)^{2/3} = \hbar^2\xi_F^2/2$. Here $\Phi(x) = 1$ if $x > 0$, and $\Phi(x) = 0$ otherwise.

The local-field correction $G(\xi)$ is related to the effective self-consistent potential $\psi(\xi)$ through $\psi(\xi) = \phi(\xi)[1 - G(\xi)]$, being therefore a measure for the deviation of the dielectric constant $\epsilon(\xi,\omega)$ from its RPA value, $\epsilon_{\rm RPA}(\xi,\omega) = 1 - \phi(\xi)\chi_0(\xi,\omega)$. In the STLS approximation it is related to the structure factor $S(\xi)$ as

$$G(\xi) = -\frac{3}{8\pi R}[\beta(\theta)\xi_F]^{-3}\int d\xi' \frac{\xi\cdot\xi'}{|\xi|^2}[S(|\xi-\xi'|)-1]\,. \tag{4}$$

Closing the self-consistent scheme, the structure factor $S(\xi)$ is related to the dielectric function $\epsilon(\xi,\omega)$ through the fluctuation-dissipation theorem as

$$S(\xi) = -\frac{\hbar}{\pi\rho\phi(\xi)}\int_0^\infty d\omega\, \mathrm{Im}\left[\frac{1}{\epsilon(\xi,\omega)}\right]. \tag{5}$$

Equations (1), (4), and (5) constitute the set that has to be self-consistently solved, to calculate $\epsilon(\xi,\omega)$ and related quantities such as pair-correlation function, structure factor, effective potential, plasmon dispersion relation, etc. In the present work we will choose units where the system can be characterized by dimensionless parameters. It is convenient to measure energies in units of E_F, frequencies in units of $E_F/\hbar$, and lengths in units of ξ_F^{-1}.

III. RESULTS

We have numerically solved these self-consistent equations for an anisotropic electron gas with $\epsilon_\infty = 1$ and $m_\parallel = m_e$, the free-electron mass, as a function of the mass ratio R, the angle θ, and the density ρ of the gas. The electron density is represented by the mean separation between the particles, $r_s = (3/4\pi\rho a_0^3)^{1/3}$, where a_0 is the Bohr radius for the free electron. The results for $R = 1$ correspond to the well-known isotropic electron gas.[3] In the case of $R \gg 1$, that is $m_\perp > m_\parallel$, we are approaching a quasi-one-dimensional system, favoring the transport along the z axis. For $R \ll 1$, the system is presenting a quasibidimensional character, since it is much easier to move carriers in the xy plane.

Figure 1 shows the plasmon dispersion relation results for $R = 5.0$, for several values of the angle and two different densities. One can notice that even for somewhat high densities ($r_s = 3$), there appears a minimum in the energy, which becomes more remarkable when the density is lowered. This minimum also increases when the angle with the z axis is enlarged, for a fixed pair of values of r_s and R.

Figure 2 represents the pair-correlation function as a function of the angle θ, for a given density and various

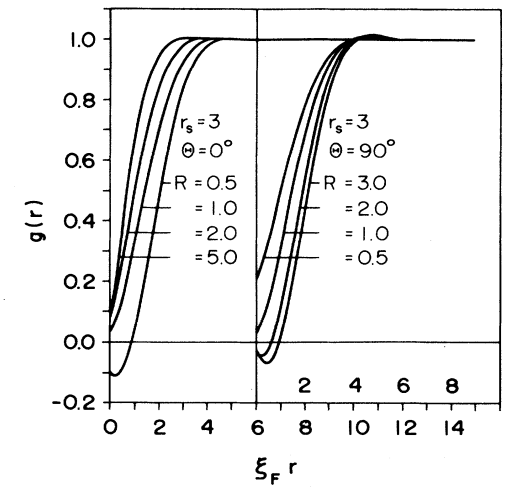

FIG. 2. Pair-correlation function $g(r)$ vs $\xi_F r$ for $r_s = 3$, $\theta = 0°$, and $\theta = 90°$ and for various values of the anisotropic mass ratio R.

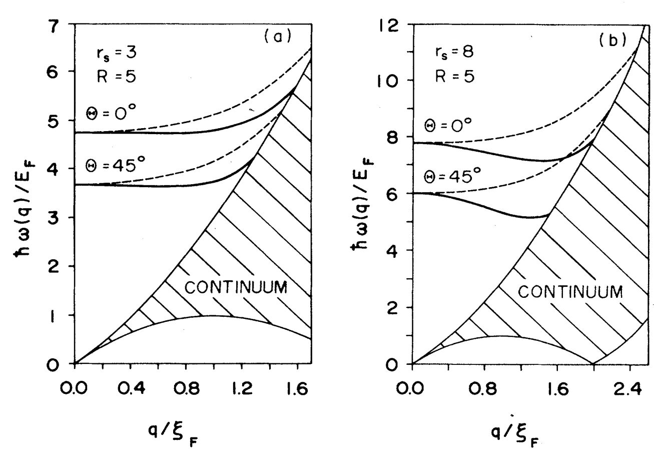

FIG. 1. Plasmon dispersion relation propagating along the axis of the strand ($\theta = 0°$) and at 45° are shown for an anisotropic mass ratio $R = 5$ and for two different electron densities; (a) $r_s = 3$ and (b) $r_s = 8$. For comparison the plasmon spectrum in the RPA is shown by dashed curves.

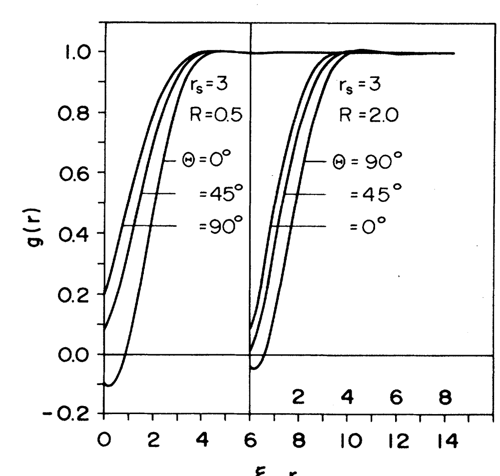

FIG. 3. Pair-correlation function $g(r)$ vs $\xi_F r$ for $r_s = 3$, $R = 0.5$, and $R = 2.0$ and for various values of θ, the angle with the axis of the strand.

values of the mass ratio R. The negative values that were found for small separation between the particles are a characteristic of STLS and should not bother us, since the values of r are then very small. Also, when the value of $g(0)$ is negative, a negative slope near $r \cong 0$ is expected, since it can be shown[7] that in this approximation the value of the derivative of $g(r)$ calculated at the origin is equal to $g(0)/a_0$. This result holds even for an anisotropic system, as can be easily proved.

Figure 3 shows the pair-correlation function for a fixed pair of values of r_s and R, and different angles. As can be seen from this figure, there is a strong difference in the behavior of the pair-correlation function at different angles, when we consider R smaller or larger than the unity. This can be explained remembering that the angle θ is measured from the z axis, and then $\theta = 0°$ means measurements along this axis, $\theta = 90°$ corresponds to the xy plane. When $R < 1$, that is $m_\perp < m_\parallel$, the system is acquiring a bidimensional character. In this case, the probability of finding the second particle at a distance r from the first is larger when the angle is large, that is, when we are examining the properties of the system almost in the xy plane, although not disconsidering the third dimension. On the other hand, for $R > 1$, we have the opposite dependence. The system now is becoming quasi-one-dimensional and therefore the probabilities should increase for low angles.

IV. CONCLUSIONS

In this paper we have shown that exchange and correlation effects are quite important in an electron gas with anisotropic effective-mass ratio. Our results mark a definite improvement over the calculations given by earlier theories using RPA. The present results lead to a more effective screening of the bare potential. It appears that we will have an improvement in the calculation of donor impurity screened in many-valley semiconductors with anisotropic masses, which is now being investigated in detail.

[1]See, for example, *Highly Conducting One-Dimensional Solids*, edited by J. T. Devreese, R. P. Evrard, and V. E. van Doren (Plenum, New York, 1979).

[2]L. A. Turkevich and R. A. Klemm, Phys. Rev. B **19**, 2520 (1979); R. L. Civiak, E. Elbaum, W. Junker, C. Gough, H. I.Kaqo, L. F. Nichols, and M. M. Labes, Solid State Commun. **18**, 1205 (1976).

[3]K. S. Singwi, P. M. Tosi, R. H. Land, and A. Sjölander, Phys. Rev. **176**, 589 (1968).

[4]V. B. Campos, O. Hipólito, and R. Lobo, Phys. Status Solidi (b) **81**, 657 (1977).

[5]J. Ruvalds, F. Brosens, F. L. Lemmens, and J. T. Devreese, Solid State Commun. **23**, 243 (1977).

[6]M. Combescot and P. Nozieres, J. Phys. C **5**, 2369 (1972).

[7]J. C. Kimball, Phys. Rev. A **7**, 1648 (1973).