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The Effect of Exchange-Correlation Holes on the Temperature Dependent Dynamic Dielectric Function of Single-Layer Quantum Wells and Coupled Nanolayers

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Abstract

In this paper, for the first time we have studied theoretically the effect of exchange-correlation holes around electrons in GaAlAs/GaAs/GaAlAs nanostructure on the temperature-dependent dynamic dielectric function of two-dimensional electron gas by employing random phase, STLS and Hubbard approximations. Also, we have investigated another interesting system which is coupled quantum wells structure. To make a good comparison and show the effect of local field, the numerical results have been compared with those obtained within RPA which considers long-range interactions and ignores exchange-correlation effects completely. We found that taking into account the exchange-correlation effects changes considerably the values of dynamic dielectric function at low electron densities at finite temperatures.

1. Introduction

Since more than two last decades nanotechnology has been received great deal of attention from researchers working in different fields of science. Nanostructures, in which incresed surface effects are responsible for outstanding properties, have been studied theoretically by quantum many-particle theory. In the heart of this theory there is dynamic dielectric function that includes necessary information about electron-electron interaction and lots of more in a many body system. The famous random phase approximation (RPA) dielectric function which considers the long-range Coulomb interaction has been used to calculate a lot of different quantities in the highly interesting quantum layers (2DEGS) so far. Although, the RPA dielectric function provides a satisfactory description of the electron gas systems, its validity is limited to high electron densities [1] though. At low electron densities, the pair correlation function obtained from

the RPA calculations is not positive for small inter-particle separations. This non-physical prediction is due to ignoring the short-range interactions. By introducing the so-called local field corrections which take into account the exchange and correlation hole around each electron, the RPA results is modified [2]. The first improvement of the RPA is the Hubbard approximation in which the short-range exchange interaction is accounted by an analytical expression for the static local field factor [3]. Also, a self-consistent local field correction containing both the exchange and correlation effects was proposed by Singwi, Tosi, Land and Sjölander (STLS) [4] who derived a relation between the static local field factor, $G(\mathbf{q})$, and static structure factor, $S(\mathbf{q})$. The static structure factor that includes the contributions from the plasmons and electron-hole excitations is related to the dielectric function through the fluctuation-dissipation theorem. Gold and Calmels [5] gave a sum-rule version of the STLS in two-dimension which was in good agreement with the full STLS and the Monte Carlo results.

In this work, we investigate the effect of short-range Coulomb interactions on the dielectric function of a GaAs-based single-layer and double-layer two-dimensional electron gas system at low densities.

2. Theory

As it is already mentioned, the STLS approximation for the dielectric function has been introduced to include the short-range exchange and correlation effects which are associated with the charge fluctuations in terms of a local field correction. The short-range interactions can be considered by calculating the dynamic dielectric function of the system, $\varepsilon(\mathbf{q},\omega)$, a functional of the Fourier transform of the pair-distribution function. This can provide a self-consistent scheme for calculating the dynamic dielectric function of a 2DEG with a sheet electron density n through these three coupled equations:

$$G(\mathbf{q}) = -\frac{1}{n}\int \frac{d\mathbf{q}'}{(2\pi)^2}\frac{\mathbf{q}.\mathbf{q}'}{q^2}\frac{v(\mathbf{q}')}{v(\mathbf{q})}\left[S(|\mathbf{q}-\mathbf{q}'|)-1\right] \quad (1)$$

$$S(\mathbf{q}) = -\frac{\hbar}{n\pi v(\mathbf{q})}\int_0^\infty d\omega \ \ \mathrm{Im}\left[\frac{1}{\varepsilon(\mathbf{q},\omega)}\right] \quad (2)$$

$$\varepsilon(\mathbf{q},\omega) = \frac{1-v(\mathbf{q})\left[1-G(\mathbf{q})\right]\chi_0(\mathbf{q},\omega)}{1+v(\mathbf{q})G(\mathbf{q})\chi_0(\mathbf{q},\omega)} \quad (3)$$

Here $\mathbf{q}$ is a 2D wave vector and $\chi_0(\mathbf{q},\omega)$ is the non-interacting two-dimensional electronic density-density response function [2]. Also, $v(\mathbf{q})$ is the Fourier transform of bare Coulomb interaction between two electrons in the lowest subband:

$$v(q) = \frac{2\pi e^2}{\varepsilon_s q}F(qL) \quad (4)$$

$F(qL)$ is the form factor of the quantum well that contained all information about geometry of system and has been calculated for an infinite rectangular quantum well as [5]:

$$F(x) = \frac{3x + 8\pi^2/x}{x^2+4\pi^2} - \frac{32\pi^4[1-exp(-x)]}{x^2(x^2+4\pi^2)^2} \quad (5)$$

where $x = qL$ and L and ε_s are the quantum layer thickness (quantum well width) and background dielectric constant, respectively. In the STLS formalism, the integral expression for $G(\mathbf{q})$ involves the static structure factor obtained from the assumption that the two-particle distribution function may be decoupled as a product of two one-particle distribution functions multiplied by the pair-correlation function. In addition to, the static structure factor is related to the dielectric function by the fluctuation-dissipation theorem and the dielectric function in turn, depends on the local field corrections. It is well-known that dielectric function can be calculated in terms of density-density response

function, Fourier transform of Coulomb potential and local field correction factor as:

$$\varepsilon(q,\omega,T)=1-\frac{v(q)\chi^0(q,\omega,T)}{1+v(q)\chi^0(q,\omega,T)G(q)} \qquad (6)$$

where $G(q)$ is the local field correction factor which contains exchange–correlation effects and $\chi^0(q,\omega)$ is the non-interacting electronic density-density response function. Of course, dynamic dielectric function for double-layer case, is a determinant.

At finite temperature, the imaginary part of χ^0 for a 2DEG system is given by [6,7]

$$\mathrm{Im}\,\chi^0(q,\omega)=N_0\frac{\sqrt{\pi t}}{2Q}\left[F_{-1/2}\left(\frac{A^+}{2}\right)-F_{-1/2}\left(\frac{A^-}{2}\right)\right] \qquad (7)$$

Here $N_0=m^*/\pi\hbar^2$ and $F_{-1/2}(x)$ is the Fermi function of order $-1/2$:

$$F_{-1/2}(x)=\frac{1}{\sqrt{\pi}}\int_0^\infty dy\frac{y^{-1/2}}{e^{(y-x)}+1} \qquad (8)$$

$A^\pm=\tilde{\mu}-(\Omega/2Q\pm Q/2)^2$ and $\tilde{\mu}=\mu/E_F$ are the dimensionless temperature, wave vector, energy and chemical potential, respectively. In a 2DEG, the dimensionless chemical potential which depends on the temperature as well as the electron density is obtained as:

$$\tilde{\mu}=t\ln(e^{1/t}-1) \qquad (9)$$

For the real part of χ^0 we have:

$$\mathrm{Re}\,\chi^0(q,\omega)=N_0\left[\frac{-1}{\exp(-\tilde{\mu}/t)+1}+\frac{Sgn(a_+)}{Q}M_t(a_+^2)-\frac{Sgn(a_-)}{Q}M_t(a_-^2)\right] \qquad (10)$$

$a_\pm=(\Omega/Q\pm Q)/2$ and the function $M_t(x)$ is defined as :

$$M_t(x)=\int_0^x d\tilde{\mu}'\frac{\sqrt{x-\tilde{\mu}'}}{4t\cosh^2\left[(\tilde{\mu}'-\tilde{\mu})/2t\right]} \qquad (11)$$

For coupled quantum layers, we need to construct dielectric matrix of the system and then we can use the determinant as the dielectric function [8] as:

$$\det\left[\varepsilon(\mathbf{q},\omega,T_1,T_2)\right]=\left(1-V_{11}(\mathbf{q})\chi_1(\mathbf{q},\omega,T_1)\right)\left(1-V_{22}(\mathbf{q})\chi_2(\mathbf{q},\omega,T_2)\right)-V_{12}(\mathbf{q})\chi_1(\mathbf{q},\omega,T_1)V_{21}(\mathbf{q})\chi_2(\mathbf{q},\omega,T_2) \qquad (12)$$

3. Results and discussion

We have calculated the dynamic dielectric function of single and double nanolayers within RPA, Hubbard and STLS approximations by employing above-mentioned theory. In all calculations the temperature is fixed and equal to Fermi temperature. Also, the density parameter is approximately 4 that makes sense to consider our system as a low density one. For this value of electron density, we know that RPA results are not reliable at all and we can focus of results from Hubbard and STLS approximations. The width of quantum wells are 20 nm and the distance between centers of quantum wells in case of double quantum wells is 50 nm. Figure 1 and 5 depict the imaginary parts of dynamic dielectric functions calculated within all approximations for single layer and double-layer cases respectively. In Figure 2 and 6 we have depicted results for the real parts of dielectric functions, again for single layer and double-layer cases, respectively. Finally, in figure 3 and 7 the norm of dielectric functions have been given within RPA, Hubbard and STLS approximations. To have an idea about the values of local filed factors in Hubbard and STLS approximations, we have provided Fig. 4 in which the local filed factors as a function of wave vector are depicted. As we see, the exchange and correlation affect seriously on the values of dynamic dielectric function of a quantum layer.

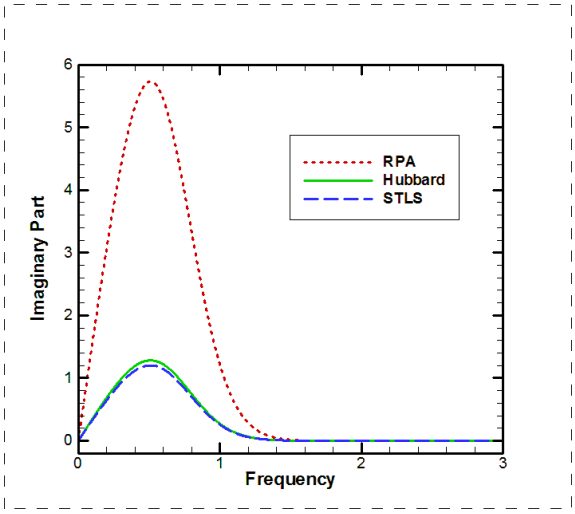

Fig. 1. Imaginary Part of dynamic dielectric function of single nanolayer within all approximations.

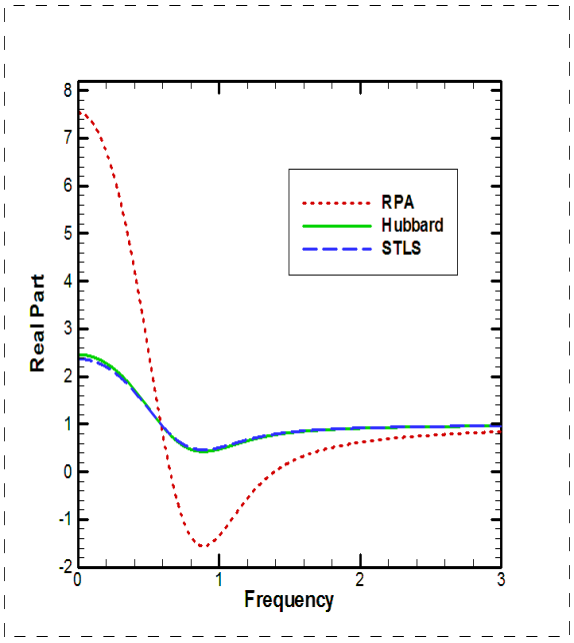

Fig. 2. Real Part of dynamic dielectric function of single nanolayer within all approximations.

4. Conclusion

In the work presented here, for the first time we have concentrated our study on the effect of exchange-correlation holes around electrons in two different interacting many-body structures, namely, single nanolayer and coupled nanolayers.

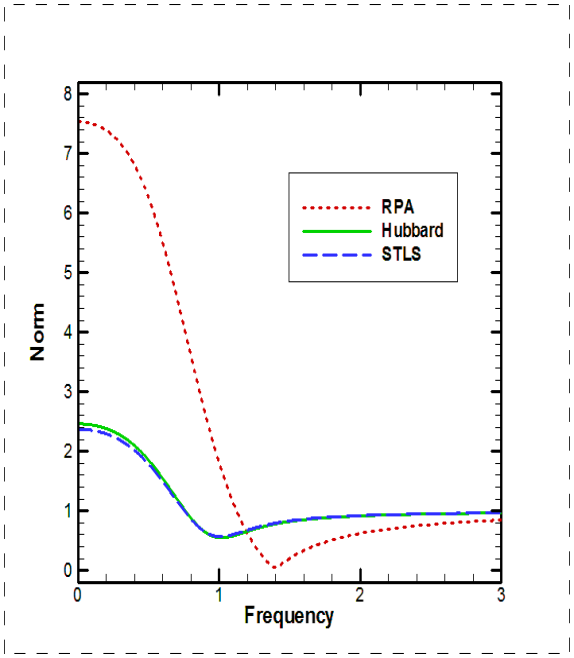

Fig. 3. Norm of dynamic dielectric function of single nanolayer within all approximations.

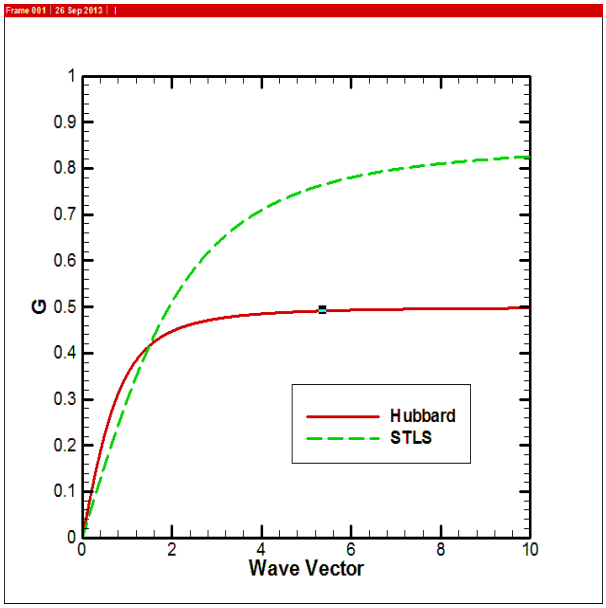

Fig. 4. Local field correction factors in Hubbard and STLS approximations.

nanolayers within all approximations.

To take into account the effect of exchange-correlation holes on the dynamic dielectrc functions of the systems, we have utilized the Hubbard and STLS approximations. Numerical results show that the correction due to local field

effect is really significant in low electron density regime.

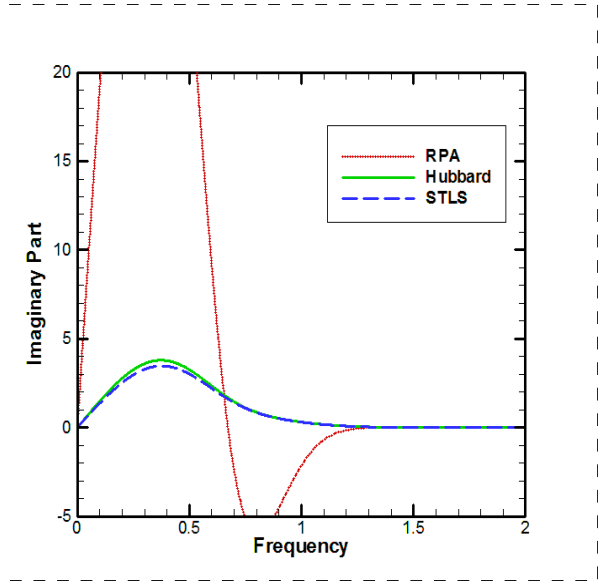

Fig. 5. Imaginary Part of dynamic dielectric function of coupled nanolayers within all approximations.

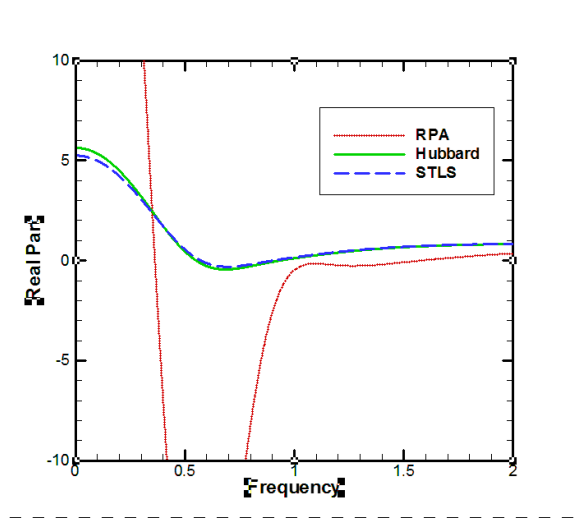

Fig.6. Real Part of dynamic dielectric function of coupled oupled

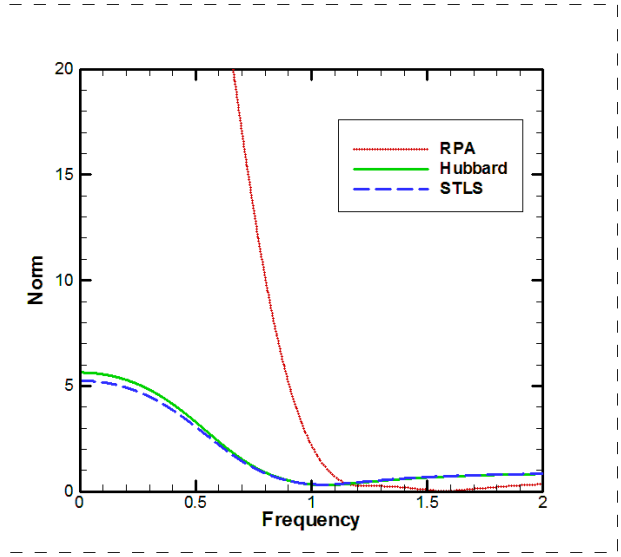

Fig. 7. Norm of dynamic dielectric function of coupled nanolayer within all approximations.

Acknowledgment

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