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Form factor for electron-electron interaction in semiconductor heterostructures

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ABSTRACT. A brief summary of the selfconsistent field method leading to a four-index matrix dielectric function, as the one of the random phase approximation, for a quasi-two-dimensional electron gas is reminded. General expressions for the form factor concerning electron-electron interaction in single heterostructures and quantum wells are derived when different dielectric constants on each side of an interface are considered and, besides, the envelope functions in the confinement direction can penetrate into the barrier regions. This problem is tightly connected with numerical calculations for multisubband transport in inversion layers and semiconductor heterostructures, as well as for other phenomena in this kind of systems where screening of involved interaction in intersubband scattering must be taken into account.

RESUMEN. En este trabajo se obtienen relaciones generales del factor de forma para la interacción electrón-electrón en heteroestructuras simples y pozos cuánticos cuando las constantes dieléctricas en cada lado de la interfase es diferente y las funciones envolventes pueden penetrar la barrera de potencial. Adicionalmente se presenta una breve descripción del método del campo autoconsistente y de la aproximación de fase aleatoria en lo que concierne al cálculo de la función dieléctrica de un gas de electrones cuasi-bidimensional. Las expresiones que aquí se presentan son útiles en el estudio de fenómenos de transporte donde participan varias sub-bandas y donde el apantallamiento involucrado juega un papel importante.

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1. INTRODUCTION

Among the electronic properties of a quasi-two-dimensional (Q2D) electron gas, formed in semiconductor heterostructures and inversion layers, transport phenomena have been widely studied both theoretically and experimentally. Most of the works developing concrete calculations has employed the so-called size-quantum-limit (SQL) approximation, where only the lowest subband and intrasubband transitions are considered. Multisubband transport, including intersubband transitions, has been treated following the quasiclassical formalism of Boltzmann transport equation (BTE) [1–11] and the quantum formalism of Kadanoff-Baym ansatz (KBA) [12–14]. Theoretical approaches have been mainly concerned with elastic scattering mechanisms [1–6, 12–14]; while inelastic scattering mechanisms have been included in a few works [7–11]. In numerical calculations carried out for momentum relaxation rates or mobilities, screening of the involved interactions has been disregarded [9, 10, 12] or considered in different ways [2, 3, 5–8, 11, 13].

Some works suggest the random-phase-approximation (RPA) result, giving a four-index matrix dielectric function (DF), to take account of the screening effect [1–4]; but the needed matrix elements of screened interaction expressed through the known matrix elements of bare interaction require the inversion of such a four-index matrix, a problem not explicitly considered in Refs. 1–4. Other works employ a strictly two-dimensional (2D) or a SQL result of the Q2D case, originally obtained in a selfconsistent field (SCF) approach, for the DF in order to consider the screening effect even in intersubband scattering [5–8, 13], what seems to be a coarse approximation, but avoid the inversion of the four-index matrix DF. A mathematical formalism has been developed to find directly the elements of the inverted four-index matrix DF [15], avoiding in this way the inversion of the generally known RPA result, but leading to a rather cumbersome procedure to take account of the screening effect.

The best DF for a Q2D electron gas to be employed in numerical calculations related to transport phenomena is the RPA result, which could be further enhanced in two ways: introducing a factor multiplying the polarizability, on the line developed by Hubbard or Singwi and Sjolander for a three dimensional (3D) electron gas [16]; or improving the polarizability itself, as Maldague did for a 2D electron gas [17]. None of that would change the four-index matrix form of DF in the Q2D case. Recently a method to invert such four-index matrix, leading to an easy procedure to take account of the screening effect, has been developed [18].

The RPA result includes the so-called form factor concerning electron-electron interaction, which takes account of the inhomogeneous character of the Q2D electron gas in the confinement direction through the envelope functions corresponding to the confining potential model [19]. It also depends on whether the Coulomb interaction is assumed to occur in an homogeneous or an inhomogeneous medium. In the former case the difference between dielectric constants on both sides of each interface is neglected, and a general expression for this form factor has been widely employed in calculations [10]. In the latter case, considering the different dielectric constants on both sides of an interface a quite general expression has been reported for inversion layers and single heterostructures (SH's) [4], but it has not been derived for quantum wells (QW's). A particular expression, assuming infinite-barrier square confining potential model (IBM), has been obtained for a QW [20]. These two expressions have in common that they have been derived for envelope functions in confinement direction which do not penetrate into the barriers at the interfaces. But consideration of finite barrier at each interface or selfconsistent calculations lead to penetration of these enveloped functions into the barrier region, a fact that can not be disregarded in calculations [19]. Since a further enhancement of the RPA result, as suggested just above, would not change the structure of this form factor, it is to the point the derivation of general expressions for SH's and QW's. The present paper aims to solve this question of both theoretical and practical interest.

2. Four-index matrix dielectric function

In the study of transport phenomena in SH's, QW's or inversion layers, we deal with a Q2D electron gas when an external field, namely the scattering field, is present. The perturbed Hamiltonian of such a system is

$$\widehat{H}(\vec{r}, z; t) = \widehat{H}_0(\vec{r}, z; t) + \widehat{V}(\vec{r}, z; t), \tag{1}$$

where the unperturbed Hamiltonian is taken in the effective mass approximation

$$\widehat{H}_0(\vec{r}, z; t) = -\frac{\hbar^2}{2m^*}\left(\nabla_{\vec{r}}^2 + \nabla_z^2\right) + U(z), \tag{2}$$

with $U(z)$ the confining potential according to the chosen model, *i.e.*, infinite triangular potential for a SH, finite-barrier square potential for a QW, selfconsistent potential for a SH or QW, etc. (see *e.g.* Ref. 19); and the perturbation is

$$\widehat{V}(\vec{r}, z; t) = V(\vec{r}, z)\exp[(i\omega + \eta)t], \tag{3}$$

with $\eta \to +0$ for adiabatic connection (after making $t \to -\infty$). Here $\vec{r} = (x, y)$ and ω is the scattering field frequency.

This perturbation is nothing else but the screened scattering potential,

$$\widehat{V}(\vec{r}, z; t) = \widehat{V}_0(\vec{r}, z; t) + \widehat{V}_1(\vec{r}, z; t), \tag{4}$$

where $\widehat{V}_0(\vec{r}, z; t)$ is the bare scattering potential (external perturbation) and $\widehat{V}_1(\vec{r}, z; t)$ is the screening potential (induced perturbation). The bare interaction corresponds to the considered scattering mechanism. Elastic scattering of electrons occurs when they interact with acoustic phonons, ion-impurities, interface roughness or some other defects; each of these mechanisms is usually modeled in the same way and one deals with static screening ($\omega = 0$). On the other hand, inelastic scattering of electrons by optical phonons depends on the starting model for this branche of lattice vibrations, leading to different interaction Hamiltonians (see, *e.g.*, Refs. 9, 11 and 19) and one must deal with dynamical screening ($\omega \neq 0$).

If the perturbation is sufficiently small (*i.e.*, $V(\vec{r}, z) \ll k_{\rm B}T$, the thermal energy of the Q2D electron gas), linearization of the equation of motion for the statistical operator and solution of the Poisson equation, relating induced perturbation with induced density of electrons, yield the following relation between 2D Fourier components of the bare interaction and the screened interaction (see, *e.g.* Ref. 20):

$$V^0_{nn'}(\vec{q}, \omega) = \sum_{l,l'} \epsilon_{nn'll'}(\vec{q}, \omega)\, V_{ll'}(\vec{q}, \omega), \tag{5}$$

which means that the matrix element of the transition between subbands n and n' due to the bare scattering potential:

$$V^0_{nn'}(\vec{q},\omega) = \int \varphi^*_{n'}(z)\, V^0(\vec{q},z;\omega)\, \varphi_n(z)\, dz, \tag{6}$$

and the matrix elements between subbands l and l' due to the screened scattering potential,

$$V^0_{ll'}(\vec{q},\omega) = \int \varphi^*_{l'}(z)\, V(\vec{q},z;\omega)\, \varphi_l(z)\, dz, \tag{7}$$

with $\varphi_l(z)$ the envelope function corresponding to $U(z)$ along the confinement direction and $\vec{q} = (q_x, q_y)$, are connected by the four-index matrix DF, whose elements are

$$\epsilon_{nn'll'}(\vec{q},\omega) = \delta_{nl}\,\delta_{n'l'} - 4\pi\chi_{nn'll'}(\vec{q},\omega), \tag{8}$$

where δ_{nl} is the Kronecker symbol and the susceptibility is

$$\chi_{nn'll'}(\vec{q},\omega) = \frac{e^2}{q\varepsilon_0 S}\Pi_{ll'}(\vec{q},\omega)\, F_{nn'll'}(\vec{q}), \tag{9}$$

where $\Pi_{ll'}(\vec{q},\omega)$ and $F_{nn'll'}(\vec{q})$ are the polarizability and the form factor, respectively, which are given by Eqs. (10) and (11), ε_0 is the static dielectric constant of the material lodging the Q2D electron gas and S the normalization area in the XY plane parallel to interfaces. The latter result could be enhanced introducing a factor multiplying the polarizability, on the line developed by Hubbard or Singwi and Sjolander for a 3D electron gas [16].

The polarizability is given by

$$\Pi_{ll'}(\vec{q},\omega) = \sum_{\vec{k}} \frac{f_{l'}(\vec{k}+\vec{q}) - f_l(\vec{k})}{E(\vec{k}+\vec{q}) + E_{l'} - E(\vec{k}) - E_l + \hbar\omega - i\eta}, \tag{10}$$

where $f_l(\vec{k})$ is the Fermi-Dirac distribution function (see, *e.g.*, Ref. 10), $E(\vec{k})$ is the quasiclassical energy associated with 2D motion of an electron with wavevector $\vec{k} = (k_x, k_y)$ and E_l is the bottom of l subband. This expression could be improved as Maldague did for a 2D electron gas [17].

The form factor concerning electron-electron interaction, obtained neglecting the difference between dielectric constants of materials forming the inversion layer, SH or QW, is given by

$$F_{nn'll'}(\vec{q}) = \int dz \int dz'\, e^{-q|z-z'|}\, \varphi^*_{n'}(z)\, \varphi_n(z)\, \varphi^*_l(z')\, \varphi_{l'}(z'), \tag{11}$$

Considering the different dielectric constants at both sides of each interface such a general expression has been reported for inversion layers and SH's [see Eq. (3.37) in Ref. 4), but it has not been derived for QW's. A particular expression, assuming infinite-barrier square confining potential, was first obtained in Ref. 20 [see Eq. (20) there].

In this way a for-index matrix DF is found using a SCF approach, but exactly the same result can also be obtained in the RPA of many-body theory, so it is usually named the RPA result.

3. FORM FACTOR FOR ELECTRON-ELECTRON INTERACTION

The derivation of a general expression for the form factor concerning electron-electron interaction, such as (11), but considering the different dielectric constants at both sides of each interface in a QW, requires the solution of an electrostatic problem, which arises when one follows the SCF approach to find the four-index matrix DF of a Q2D electron gas. (see, *e.g.*, Ref. 20).

The Poisson equation relating induced perturbation with induced density of electrons results in the following equation for the 2D Fourier component of the screening potential:

$$\widehat{\mathcal{L}}\, V^1(z) = -4\pi J(z), \tag{12}$$

where the lineal differential operator is

$$\widehat{\mathcal{L}} = \frac{d^2}{dz^2} - q^2 \tag{13}$$

and the induced charge density is given by:

$$J(z) = \frac{e^2}{\varepsilon(z) S} \sum_{\vec{k},\, l} \sum_{\vec{k'},\, l'} \langle \vec{k'},\, l' | \hat{\rho}_1 | \vec{k},\, l \rangle \cdot \varphi_l^*(z)\, \varphi_{l'}(z) \cdot \delta_{\vec{k'}, \vec{k}+\vec{q}}\,, \tag{14}$$

with S the normalization area in XY plane, $\hat{\rho}_1$ the non-equilibrium part of the statistical operator and

$$\varepsilon(z) = \begin{cases} \varepsilon_w, & 0 < z < d \quad \text{(inside the QW);} \\ \varepsilon_b, & z < 0 \quad \text{and} \quad z > d \quad \text{(in the barriers).} \end{cases} \tag{15}$$

Equation (12) must be solved together with the boundary conditions at $z \to \pm\infty$ and the matching conditions at $z = 0$ and $z = d$:

$$V^1(\pm\infty) = 0, \tag{16}$$

$$V^1(0^-) = V^1(0^+), \qquad V^1(d^-) = V^1(d^+), \tag{17}$$

$$\varepsilon_b \frac{d}{dz} V^1(0^-) = \varepsilon_w \frac{d}{dz} V^1(0^+), \qquad \varepsilon_w \frac{d}{dz} V^1(d^-) = \varepsilon_b \frac{d}{dz} V^1(d^+). \tag{18}$$

The solution of the mathematical problem (12) with (16)–(18) is sought employing the Green function (GF) method. Thus one has

$$V^1(z) = \int dz'\, J(z')\, G(z, z'), \tag{19}$$

where the GF have to satisfy the following equation:

$$\widehat{\mathcal{L}}\, G(z, z') = -4\pi \delta(z - z'), \tag{20}$$

together with the same kind of boundary and matching conditions:

$$G(\pm\infty, z') = 0, \tag{21}$$

$$G(0^-, z') = G(0^+, z'), \qquad G(d^-, z') = G(d^+, z'), \tag{22}$$

$$\varepsilon_b \frac{d}{dz} G(0^-, z') = \varepsilon_w \frac{d}{dz} G(0^+, z'), \qquad \varepsilon_b \frac{d}{dz} G(d^-, z') = \varepsilon_w \frac{d}{dz} G(d^+, z'). \tag{23}$$

One looks for the solution of (9)–(12) in the form

$$G(z, z') = \frac{2\pi}{q} \Gamma(z, z'), \tag{24}$$

where

$$\Gamma(z, z') = \begin{cases} \Gamma_{\mathrm{L}}(z, z'), & z' < 0 \\ \Gamma_{\mathrm{W}}(z, z'), & 0 < z' < d \\ \Gamma_{\mathrm{R}}(z, z'), & z' > d. \end{cases} \tag{25}$$

The GF can be interpreted as reflecting the interaction between a source charge placed at z' and a test charge placed at z. The presence of the interfaces is taken into account by means of the two image charges corresponding to the source charge. The test charge interacts with an image charge only if they are located at different media and, besides, at different sides of the interface giving rise to the latter. Notice that here one is dealing with dielectrics and there are only two images of the source, which are due to the polarization of the media, but not a series of images as in the case of conductors.

This way when the source charge is on the left side of the QW ($z' < 0$):

$$\Gamma_{\mathrm{L}}(z, z') = \begin{cases} e^{-q|z-z'|} + A_{\mathrm{L}} e^{q(z+z')}, & z < 0; \\ B_{\mathrm{L}} e^{-q(z-z')} + C_{\mathrm{L}} e^{q(z-z'-2d)}, & 0 < z < d; \\ D_{\mathrm{L}} e^{-q(z-z')}, & z > d; \end{cases} \tag{26}$$

where the constants are found from the matching conditions (22) and (23)

$$A_{\mathrm{L}} = \frac{1}{E} \left(\varepsilon_b^2 - \varepsilon_w^2\right) \left(1 - e^{-2qd}\right), \tag{27}$$

$$B_{\mathrm{L}} = \frac{2}{E} \varepsilon_b \left(\varepsilon_w + \varepsilon_b\right), \tag{28}$$

$$C_{\mathrm{L}} = \frac{2}{E} \varepsilon_b \left(\varepsilon_w - \varepsilon_b\right) e^{2qz'}, \tag{29}$$

$$D_{\mathrm{L}} = \frac{4}{E} \varepsilon_b \varepsilon_w, \tag{30}$$

with

$$E = \left(\varepsilon_b + \varepsilon_w\right)^2 - \left(\varepsilon_b - \varepsilon_w\right)^2 e^{-2qd}. \tag{31}$$

When the source charge is inside of the QW ($0 < z' < d$):

$$\Gamma_{\mathrm{W}}(z,z') = \begin{cases} A_{\mathrm{W}} e^{q(z-z')}, & z < 0; \\ e^{-q|z-z'|} + B_{\mathrm{W}} e^{-q(z+z')} + C_{\mathrm{W}} e^{q(z+z'-2d)}, & 0 < z < d; \\ D_{\mathrm{W}} e^{-q(z-z')}, & z > d; \end{cases} \tag{32}$$

where, from the matching conditions,

$$A_{\mathrm{W}} = \frac{2}{E}\varepsilon_w \left[(\varepsilon_w + \varepsilon_b) + (\varepsilon_w - \varepsilon_b)\, e^{2q(z'-d)}\right], \tag{33}$$

$$B_{\mathrm{W}} = \frac{1}{E}(\varepsilon_w - \varepsilon_b)\left[(\varepsilon_w + \varepsilon_b) + (\varepsilon_w - \varepsilon_b)\, e^{2q(z'-d)}\right], \tag{34}$$

$$C_{\mathrm{W}} = \frac{1}{E}(\varepsilon_w - \varepsilon_b)\left[(\varepsilon_w + \varepsilon_b) + (\varepsilon_w - \varepsilon_b)\, e^{-2qz'}\right], \tag{35}$$

$$D_{\mathrm{W}} = \frac{2}{E}\varepsilon_w \left[(\varepsilon_w + \varepsilon_b) + (\varepsilon_w - \varepsilon_b)\, e^{-2qz'}\right]. \tag{36}$$

Finally, when the source charge is on the right side of the QW ($z' > d$):

$$\Gamma_{\mathrm{R}}(z,z') = \begin{cases} A_{\mathrm{R}} e^{-q(z'-z)}, & z < 0; \\ B_{\mathrm{R}} e^{-q(z-z'+2d)} + C_{\mathrm{R}} e^{-q(z'-z)}, & 0 < z < d; \\ e^{-q|z-z'|} + D_{\mathrm{R}} e^{-q(z+z'-2d)}, & z > d; \end{cases} \tag{37}$$

where, from the matching conditions,

$$A_{\mathrm{R}} = \frac{4}{E}\varepsilon_w \varepsilon_b, \tag{38}$$

$$B_{\mathrm{R}} = \frac{2}{E}\varepsilon_b(\varepsilon_w - \varepsilon_b)e^{-2q(z'-d)}, \tag{39}$$

$$C_{\mathrm{R}} = \frac{2}{E}\varepsilon_b(\varepsilon_w + \varepsilon_b), \tag{40}$$

$$D_{\mathrm{R}} = \frac{1}{E}\left(\varepsilon_b^2 - \varepsilon_w^2\right)\left(1 - e^{-2qd}\right). \tag{41}$$

Notice that if one takes the limit case $d \to 0$ and $\varepsilon_w \to \varepsilon_b$ the following values are obtained: $A_{\mathrm{L}} = 0$, $B_{\mathrm{L}} = 1$, $C_{\mathrm{L}} = 0$, $D_{\mathrm{L}} = 1$; $A_{\mathrm{W}} = 1$, $B_{\mathrm{W}} = 0$, $C_{\mathrm{W}} = 0$, $D_{\mathrm{W}} = 1$; $A_{\mathrm{R}} = 1$, $B_{\mathrm{R}} = 0$, $C_{\mathrm{R}} = 1$, $D_{\mathrm{R}} = 0$. This means that from (32), (26) or (37) one recovers the homogeneous case.

Following the GF method, as it has just been employed for a QW, one can find for a SH that the GF corresponding to the electrostatic problem similar to (12) and (16)–(18) (now one must omit matching conditions at $z = d$ since this interface does not exit) has exactly the form given by (24), but now:

$$\Gamma(z,z') = \begin{cases} \Gamma_-(z,z'), & z' < 0; \\ \Gamma_+(z,z'), & z' > 0. \end{cases} \tag{42}$$

When the source charge is at left from the interface ($z' < 0$):

$$\Gamma_-(z,z') = \begin{cases} e^{-q|z-z'|} + A_- e^{q(z+z')}, & z' < 0; \\ B_- e^{q(z'-z)}, & z' > 0; \end{cases} \tag{43}$$

where

$$A_- = \frac{\varepsilon_b - \varepsilon_w}{\varepsilon_b + \varepsilon_w}, \qquad B_- = \frac{2\varepsilon_b}{\varepsilon_b + \varepsilon_w}. \tag{44}$$

Finally, when the source charge is at right from the interface ($z' > 0$):

$$\Gamma_-(z,z') = \begin{cases} C_+ e^{q(z-z')}, & z' < 0; \\ e^{q|z-z'|} + D_+ e^{q(z+z')}, & z' > 0 \end{cases} \tag{45}$$

where

$$C_+ = \frac{2\varepsilon_w}{\varepsilon_b + \varepsilon_w}, \qquad D_+ = \frac{\varepsilon_w - \varepsilon_b}{\varepsilon_b + \varepsilon_w}. \tag{46}$$

Notice that if one takes the limit case $\varepsilon_w \to \varepsilon_b$ the following values are obtained: $A_- = 0$, $B_- = 1$; $C_- = 1$, $D_- = 0$. This means that from (43) or (45) one recovers the homogeneous case.

Finally, remark that taking the limit $d \to \infty$ from (26) obtains (43), while from (32) or (37) one obtains (45).

Following the SCF approach straightforward calculations lead to

$$F_{nn'll'}(q) = \int_{-\infty}^{+\infty} dz \int_{-\infty}^{+\infty} dz' \; \Gamma(z,z';q)\, \varphi^*_{n'}(z)\, \varphi_n(z)\, \varphi^*_l(z')\, \varphi_{l'}(z), \tag{47}$$

which is the more general expression for the form factor one can write to employ any envelope functions in the confinement direction. Of course, the function $\Gamma(z,z';q)$ have to be specified in accordance with the results presented just above in this section.

4. Conclusions

In this paper we have derived general expressions for the form factor concerning electron-electron interaction in SH's and QW's when different dielectric constants at each side of an interface are considered and, besides, the envelope functions in the confinement direction can penetrate into the barrier regions. For this purpose we have employed the GF method together with the image method to solve the electrostatic problem arising in the confinement direction; these methods seems to be the more suitable ones, as will be discussed elsewhere.

This problem is connected not only with multisubband transport in semiconductor heterostructures or inversion layers, but also with any calculation concerning phenomena in Q2D systems where the screening of involved interactions in intersubband scattering must be taken into account. Actual calculations are in progress in our group and will be presented in a further paper.

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