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The finite-temperature photoluminescence correlation function in semiconductor heterostructures

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Abstract. We report the inclusion of temperature effects on the Mahan-Nozières-De Dominicis framework to study both many-body and temperature effects in photoluminescence spectra of doped semiconductors. The electronic part of the correlation function characterizes the photoluminescence spectra. We have treated the optical valence hole as a localized scattering potential center and studied effects of the electron-hole interaction enhancement on the photoluminescence spectra leading to the appearance of shake-up structures. We also have identified a term in the correlation function which represents the finite-temperature contribution to the intensities of the shake-up structures. The method is used to study the magnetophotoluminescence of modulation-doped quantum wells with a weak periodic lateral potential.

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1 Introduction

Recent experimental and theoretical studies of the photoluminescence (PL) spectra of n-doped low-dimensional semiconductors have attracted considerable interest due to the appearance of many-body effects, as *e.g.* those that give origin to the Fermi-edge singularity (FES) [1]. The application of a high magnetic field perpendicular to the plane of a quasi-two-dimensional doped system leads to the investigation of the many-body effects on PL spectra in the regime of quantum Hall effect (QHE) [2–5]. Some experiments show new many-body effects related to the spin resolution in PL spectra of a system in which the $\nu = 1$ quantum Hall regime is achieved [3]. In order to study such effects from a theoretical point of view, a zero-temperature formulation has been carried out where the authors have associated these many-body effects to the spin shake-up processes [6]. Besides, some PL experiments [2] also show finite-temperature effects on the shake-up processes [4] in the integer quantum Hall regime without a resolution of the electronic spin. A further analysis shows, on the other hand, the influence of the finite valence-hole effective mass on the PL spectra in the quantum Hall regime [5]. All these works reflect both a strong experimental and theoretical interests in the finite-temperature PL spectra studies of quasi-two-dimensional (Q2D) systems under a perpendicular magnetic field. Our main motivation here is to extend to the finite-temperature the Mahan-Nozières-De Dominicis (MND) formulation in order to be able to study both the many-body and temperature effects on PL spectra of Q2D systems.

We would like to point out that some many-body finite-temperature approaches have been successfully used to study PL spectra in modulation-doped quantum wells [7,8]. The one developed by Ohtaka and Tanabe (OT) is based on the Fermi golden rule. It involves a careful description of temperature effects but it becomes rather cumbersome from the practical point of view while we are looking for an approach where we may describe, in a simpler manner, both many-body and temperature effects. We have chosen to look for an extension of the zero temperature MND formalism which has already proved to be a satisfactory approach with a rigorous description of the physical processes besides its practical manageability [9–13]. For this reason, the aim of this work is to present a solid procedure to include the effects of temperature on the emission MND correlation function, the key point in the description of PL spectra. We have adopted a procedure similar to the one followed by Mahan [11] to calculate the zero-temperature scattering matrix in the second quantization scheme. It must be stressed that the main goal of this paper is to present a method which properly clarifies the calculation of PL spectra at finite-temperature within a second quantization scheme. Subsequently, the method is applied to a particular quasi-two-dimensional system in which the spin of the electrons is not resolved. Studies

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of PL spectra of spin systems should require a method which takes into account the spin-spin excitation effects.

The paper is organized as follows. In Section 2, our extension to finite temperatures of the MND current-current correlation function describing PL spectra is presented. We discuss new terms appearing in the correlation function and we study its $T \to 0$ limit. In Section 3 we apply our theory to a Q2D system under both a perpendicular magnetic field and a weak periodic modulation potential and comparing our results with the available experimental information [14]. The effects of the electron-hole interaction enhancement in the PL spectra of the system are investigated as well.

2 Extension to the finite temperature of the MND formulation for PL

The current-current correlation function which describes the PL spectra is written here within an one-body picture [10], in which the Coulomb interaction between conduction electrons produces quasiparticles near the Fermi surface. We assume that electron-electron interaction can be taken into account in a phenomenological way so that we already work with quasiparticles. In this description, each quasiparticle only interacts with a scattering potential associated to a valence hole. Moreover, the hole potential is assumed to be switched on infinitely fast so that, one consider the electron-hole interaction to be instantaneously screened by charge density fluctuations of the electrons in the Fermi sea.

We must point out that, in many recent reports a crucial factor which allowed the experimental observation of the FES in PL was the localization of the valence hole by a form of disorder, typically alloy fluctuations in $In_xGa_{1-x}As$ wells [15]. Moreover, in a quasi-one-dimensional electron gas the FES was also easier observed when the valence hole were localized by acceptor impurities [16]. In order to compare our theoretical results with the experimental situation, we are going to treat the optical created hole as a scattering potential center localized in the valence band.

We start with the current-current correlation function $E(\tau)$, whose Fourier transformed characterizes the PL spectra of doped systems at finite temperature, given by

$$E(\tau) = \mathrm{e}^{\tau\varepsilon_h} \sum_{\lambda,\lambda'} m_\lambda m^*_{\lambda'} L_{\lambda,\lambda'}(\tau), \tag{1}$$

with

$$L_{\lambda,\lambda'}(\tau) = \left\langle c^+_\lambda(\tau) S(\tau)\, c_{\lambda'} \right\rangle, \tag{2}$$

which characterizes the electronic part of the correlation function related to emission. In the above equations, the time (usually labeled as τ) becomes a complex quantity, *i.e.*, $\tau = it$, and the bracket $\langle\rangle$ stands for the thermodynamic average. The transition-matrix element m_λ is given by

$$m_\lambda = \sum_k M_k \left\langle \lambda \right| k \left\rangle \right., \tag{3}$$

where $\left\langle \lambda \right| k \left\rangle \right.$ (Mahan excitons) is the overlap between the initial single-particle state $|\lambda\rangle$ and the final single-particle state $|k\rangle$. Such overlaps can be calculated solving the Wannier equation [13] which takes into account the electron-hole interaction V_{e-h}. In the calculation, we consider a photocreated hole localized in the valence band with energy ε_h and a contact electron-hole interaction which switches on already screened. Moreover, $M_k = \mathcal{M}_0 \left\langle k \right| h \left\rangle \right.$ are the single-particle transition matrix elements, which are characterized by the localized valence hole state $|h\rangle$ and the momentum matrix element $\mathcal{M}_0$ (taken as a constant in this work).

For PL process, the time-evolution operator $S(\tau)$ is defined as

$$S(\tau) = \mathrm{e}^{\tau \hat{K}_h} \mathrm{e}^{-\tau \hat{K}_g}, \tag{4}$$

where the Hamiltonian $\hat{K}_g = \sum_k \xi_k c^+_k c_k$ ($\hat{K}_h = \sum_\lambda \xi_\lambda c^+_\lambda c_\lambda$) describes the many-particle system in the absence (presence) of the core hole. The operator $c_\lambda(c^+_\lambda)$ destroys (creates) a relaxed electron in the conduction band state $|\lambda\rangle$ with a single-particle energy $\xi_\lambda = (\epsilon_\lambda - \mu)$, where μ is the chemical potential. On the other hand, $c_k(c^+_k)$ destroys (creates) an electron in the conduction band state $|k\rangle$, with single-energy $\xi_k = (\epsilon_k - \mu)$. Noticed that the single-particle basis $\{|k\rangle\}$ characterizes the many-particle system in the absorption (emission) initial (final) state, *i.e.*, without the core-hole potential. On the other hand, the single-particle basis $\{|\lambda\rangle\}$ describes the many-particle system in the emission (absorption) initial (final) state, *i.e.*, when the electron-hole potential is present.

In order to examine the one-body approximation, Mahan [11] used scattering theory to write out the zero-temperature expression of $E(\tau)$ in terms of single-particle quantities. With such a procedure, he showed that the emission expression of Combescot and Nozières (CN) [17] can also be derived by scattering theory. Following the CN formulation, the extension of the optical correlation function to finite temperature is a very difficult task due to the fact that we have to deal with a linear combination of different Slater determinants [18]. So in this work we will avoid the CN formulation, because the Mahan's rederivation of the optical correlation function leads to an easier extension to finite-temperature.

In order to obtain the electronic parts of both $E(\tau)$ at finite temperature, we expand the expression of $S(\tau)$ as

$$S(\tau) = \sum_{n=0}^{\infty} \left(\frac{-1}{\hbar}\right)^n \frac{1}{n!} \times \int_0^\tau \mathrm{d}\tau_1 ... \int_0^\tau \mathrm{d}\tau_n T_\tau \left[V(\tau_1)...V(\tau_n)\right]. \tag{5}$$

In the above equation, the time-dependent electron-hole potential $V(\tau_n)$ can be written in the single-state basis $\{|\lambda\rangle\}$

$$V(\tau_n) = \sum_{\lambda_1,\lambda_2} V_{e-h}(\lambda_1,\lambda_2) c_{\lambda_1}(\tau_n) c^+_{\lambda_2}(\tau_n).$$

In the expansion of the zero-temperature expression of $S(\tau)$, Mahan kept only the exciton terms and ignored the terms coming from the conduction electron-hole pairs in the electron gas, which provoke the Anderson orthogonalization catastrophe. In other words, he kept only the terms in the series represented by connected diagrams and ignored all the disconnected diagrams. The hole self-energy effects in the correlation functions $E(\tau)$ were neglected. We are going to follow similar steps to calculate the electronic part of both $E(\tau)$ at finite temperature. This is possible because the temperature does not include any other type of diagrams, *i.e.*, the diagrams appearing in the finite-temperature expansion of $S(\tau)$ are those which already exist at zero-temperature.

We have performed the expansion of the S-matrix in equation (2), keeping only the terms which correspond to the connected diagrams. After some algebra, we obtain the exact solution for $L_{\lambda,\lambda'}(\tau)$, given by

$$L_{\lambda,\lambda'}(\tau) = \mathcal{L}^1_{\lambda,\lambda'}(\tau) + \mathcal{L}^2_{\lambda,\lambda'}(\tau) \tag{6}$$

where

$$\mathcal{L}^1_{\lambda,\lambda'}(\tau) = \left\langle \lambda' \left| \mathrm{e}^{\tau \hat{K}_h} \hat{P}^E \hat{X}^E \hat{P}^E \right| \lambda \right\rangle \tag{7}$$

and

$$\mathcal{L}^2_{\lambda,\lambda'}(\tau) = \left\langle \lambda' \left| \mathrm{e}^{\tau \hat{K}_h} \hat{P}^E \left[1 - \hat{\Phi}^E \hat{X}^E \hat{P}^E \right] \right| \lambda \right\rangle . \tag{8}$$

The operator $\hat{P}^E$ in equation (7) is the projection operator on the initial single-particle states of the emission process

$$\hat{P}^E = \sum_\lambda \left| \lambda \right\rangle n^T_\lambda \left\langle \lambda \right|, \tag{9}$$

where n^T_λ is the Fermi-Dirac distribution function

$$n^T_\lambda = \frac{1}{1 + \mathrm{e}^{\beta \xi_\lambda}} \cdot \tag{10}$$

The time-evolution operator for emission $\hat{\Phi}^E$ in equation (8), has an S-matrix form

$$\hat{\Phi}^E = \hat{\Phi}^E(\tau) = \mathrm{e}^{\hat{K}_h \tau} \mathrm{e}^{-\hat{K}_g \tau}. \tag{11}$$

The last ingredient in equations (7, 9) is the operator

$$\hat{X}^E = 1 + \left[1 - \hat{P}^E (1 - \hat{\Phi}^E) \right]^{-1} \hat{P}^E (1 - \hat{\Phi}^E), \tag{12}$$

which give rise to the replacement transitions.

We would like to emphasize that, apart from the approximation of neglecting hole self-energy effects (*i.e.* to neglect disconnected diagrams, or hole-recoil effect), the correlation function equation (6) is exact, because the expansion of $S(\tau)$ can be exactly summed. Moreover, the temperature dependence of the hole self-energy could be important to the PL spectra and, as far as we know, there is no previous theoretical study of temperature dependence of hole spectral functions. In such a study, one could proper describe the temperature behavior in experiments involving PL of doped quantum wells. However, in the present work we will not consider the hole self-energy effects since our main purpose is to investigate the new finite temperature contributions coming from the electronic part of the PL correlation function.

Equation (6) do not include any valence-hole scattering, since we are considering an immobile hole. This simplifies the identification of the disconnect diagrams in the $S(\tau)$ expansion, and allows one to find out the electronic part of the optical correlation function. If we consider the valence-hole scattering, *i.e.*, the case of mobile valence holes, the exact connected-diagram summation becomes extremely difficult.

Finally, in the following subsections we will analyze the terms $\mathcal{L}^1_{\lambda,\lambda'}(\tau)$ and $\mathcal{L}^2_{\lambda,\lambda'}(\tau)$ contributing to our expression for the PL spectra. In order to do so, we are going to study the $T \to 0$ limit of these terms and compare the results with the well known MND zero-temperature emission expressions.

2.1 T→ 0 limit of $\mathcal{L}^1_{\lambda,\lambda'}(\tau)$ and $\mathcal{L}^2_{\lambda,\lambda'}(\tau)$

At zero temperature, the Fermi-Dirac distribution function n^0_λ, as given by equation (10), can only take two values: $n^0_\lambda = 0$ for non-occupied states, and $n^0_\lambda = 1$ for occupied states. Thus, at zero temperature the equality $n^0_\lambda = (n^0_\lambda)^2$ holds so that, the quantity $\hat{P}^E$ in equation (9) becomes an unitary operator

$$\hat{P}^E = \left(\hat{P}^E \right)^2. \tag{13}$$

Notice that this holds only for those cases where the temperature is strictly zero.

Using the unitarity property of the projection-like operator $\hat{P}^E$, the $T \to 0$ limit of the operator $\hat{X}^E$ can be written as

$$\hat{X}^0 = \lim_{T \to 0} \hat{X}^E = (\hat{P}^E \hat{\Phi}^E)^{-1} \hat{P}^E, \tag{14}$$

where we have used the identity

$$(\hat{P}^E \hat{\Phi}^E)^{-1} \hat{P}^E \hat{\Phi}^E = 1. \tag{15}$$

Therefore, according to equation (14), the zero-temperature expression for $\mathcal{L}^1_{\lambda,\lambda'}(\tau)$ is given by

$$\lim_{T \to 0} \mathcal{L}^1_{\lambda,\lambda'}(\tau) = \left\langle \lambda' \left| \mathrm{e}^{\mathrm{i}t\xi_{\lambda'}} \hat{P}^E (\hat{P}^E \hat{\Phi}^E)^{-1} \hat{P}^E \right| \lambda \right\rangle, \tag{16}$$

while, from equation (15), we have

$$\lim_{T \to 0} \mathcal{L}^2_{\lambda,\lambda'}(\tau) = 0. \tag{17}$$

The term $\mathcal{L}^2_{\lambda,\lambda'}(\tau)$, at zero temperature, vanishes and, according to equation (16), the zero-temperature PL spectra is the Fourier transform of

$$L^0(t) = \mathrm{e}^{\mathrm{i}t\varepsilon_h} \sum_{\lambda,\lambda'} M_\lambda M^*_{\lambda'} \left\langle \lambda' \left| \mathrm{e}^{\mathrm{i}t\xi_{\lambda'}} \hat{P}^E (\hat{P}^E \hat{\Phi}^E)^{-1} \hat{P}^E \right| \lambda \right\rangle \tag{18}$$

which is the MND expression given in reference [11]. Such expression has been successfully used in calculations of the zero-temperature PL spectra of quasi-2-dimensional doped systems [12]. Thus one can interpret it as the transition of a relaxed conduction-electron to the valence band with an instantaneous rearrangement of the Fermi sea to the new states in which the electrons do not feel the hole potential. Such transitions are mediated by the exchange processes of electrons inside the Fermi sea, *i.e.*, they are replacement transitions. These exchange processes are characterized by the operator $(\hat{P}^E\hat{\Phi}^E)^{-1}$ of equation (18).

One can see from equations (16) and (17) that the results of the finite-temperature extension of the MND PL expressions are analogous to the absorption case [19], where a new contribution due to the finite values of temperature appears. In the PL case, such new contribution is represented by equation (8) and it must be interpreted in the same way as done in the absorption case.

2.2 Comparison between finite-temperature absorption and emission expressions

Let us discuss the meaning of each term in $L_{\lambda,\lambda'}(\tau)$. For convenience, we write here the absorption counterpart of $\mathcal{L}^1_{\lambda,\lambda'}(\tau)$ and $\mathcal{L}^2_{\lambda,\lambda'}(\tau)$. They are given by $\mathcal{F}^1_{k,k'}(\tau) = \langle k|\mathrm{e}^{-\tau\hat{K}_g}(1-\hat{P}^A)\ \hat{\Phi}^A\hat{X}^A(1-\hat{P}^A)|k'\rangle$ and $\mathcal{F}^2_{k,k'}(\tau) = \langle k|\mathrm{e}^{-\tau\hat{K}_h}(1-\hat{P}^A)[1-\hat{X}^A(1-\hat{P}^A)]|k'\rangle$, respectively. These absorption results have been taken from reference [19]. Here the operators $\hat{P}^A = \sum_k |k\rangle n_k^T\langle k|$, $\hat{\Phi}^A = \mathrm{e}^{\hat{K}_g\tau}\mathrm{e}^{-\hat{K}_h\tau}$ and $\hat{X}^A = 1 + [1-\hat{P}^A(1-\hat{\Phi}^A)]^{-1}\hat{P}^A(1-\hat{\Phi}^A)$ are the absorption counterpart of the emission expressions given by equations (9-12). At zero temperature, $\mathcal{L}^2_{\lambda,\lambda'}(\tau)$ and $\mathcal{F}^2_{k,k'}(\tau)$ vanish. At this limit, we can recover the zero-temperature results obtained by Mahan [11]. $\mathcal{F}^1_{k,k'}(\tau)$ contains two different kind of transitions. The first one is associated with the first term of the operator $\hat{X}^A$, *i.e.*, the identity operator, which gives rise to the direct scattering of an injected electron above the Fermi surface with an instantaneous rearrangement of the Fermi sea to the new state in which electrons feel the hole potential. The second one, is associated with the operator $[1-\hat{P}^A(1-\hat{\Phi}^A)]^{-1}\hat{P}^A(1-\hat{\Phi}^A)$, which gives rise to scattering mediated by exchange processes provided by the occupied states inside the Fermi sea. These two kind of transitions occur even at zero-temperature and they were named by Friedel [20] as the direct and replacement transitions, respectively. The emission counterpart of $\mathcal{F}^1_{k,k'}(\tau)$ is the term which survives at zero temperature, *i.e.* $\mathcal{L}^1_{\lambda,\lambda'}(\tau)$. Even at finite temperature, one can interpret $\mathcal{L}^1_{\lambda,\lambda'}(\tau)$ as the transition of a relaxed conduction-electron to the valence band with an instantaneous rearrangement of the Fermi sea to the new states in which the electrons do not feel the hole potential. Such transitions are mediated by exchange processes of electrons inside the Fermi sea, *i.e.*, they are replacement transitions. These exchange processes are described by the operator X^E. At zero-temperature limit, the terms $\mathcal{F}^1_{k,k'}(\tau)$ and $\mathcal{L}^1_{\lambda,\lambda'}(\tau)$ become the zero-temperature expressions obtained by Mahan.

The term $\mathcal{F}^2_{k,k'}(\tau)$ represents new physical processes adding interesting features related to temperature effects. The first one has been interpreted as the matrix elements which represent the thermally created electron-hole pairs at energies in the vicinity the Fermi level. The second one represents the replacement transitions of the photoexcited electrons to conduction-band states bellow the Fermi level, which are empty due to thermal excitation. On the other hand, its emission counterpart, *i.e.* $\mathcal{L}^2_{\lambda,\lambda'}(\tau)$, can be interpreted as those transitions to the valence band whose exchange processes are provided by occupied states belonging to the thermally created electron-hole pairs at energies around the Fermi level. When the temperature is strictly zero, the Fermi surface has a sharp edge and the electron-hole-pairs region disappears. In this situation, the peculiar replacement transitions represented by $\mathcal{F}^2_{k,k'}(\tau)$ and $\mathcal{L}^2_{\lambda,\lambda'}(\tau)$ do not exist. These replacement transitions contributing to the optical spectra only occur at finite temperature.

2.3 PL spectra written in the final basis set

In order to arrive to the one-body approximation, we can write the finite-temperature emission correlation function (6) in the basis set of the electronic final states [11]. Thus, using the definition of m_λ, given in equation (3), into equation (6), one easily obtains the total frequency dependent PL spectra as a sum of two terms

$$E(\omega) = E_1(\omega) + E_2(\omega). \tag{19}$$

The first term, $E_1(\omega)$, depends on $\mathcal{L}^1_{\lambda,\lambda'}(\tau)$ which survives at zero temperature

$$E_1(\omega) = 2\mathrm{Re}\left\{\int_0^\infty \mathrm{d}\tau\ \mathrm{e}^{\tau(\omega+\varepsilon_h-\mathrm{i}\eta)} \times \sum_{kk'}\left[M_k\mathcal{G}^1_{k,k'}(\tau)M^*_{k'}\right]\right\}, \tag{20}$$

where $\mathcal{G}^1_{k,k'}(\tau)$ is the vertex correction function defined as

$$\mathcal{G}^1_{k,k'}(\tau) = \sum_{\lambda,\lambda'}\mathrm{e}^{\tau\xi_\lambda}n^T_\lambda n^T_{\lambda'}\langle k|\ \lambda\rangle\,\mathcal{X}_{\lambda,\lambda'}(\tau)\,\langle\lambda'|\,k'\rangle\,. \tag{21}$$

$\mathcal{X}_{\lambda,\lambda'}(\tau)$ are the matrix elements of the operator $\hat{X}^E$ in the initial electronic basis set. One can verify that $\mathcal{X}_{\lambda,\lambda'}(\tau)$ is given by

$$\mathcal{X}_{\lambda,\lambda'}(\tau) = \delta_{\lambda,\lambda'} + \left(n^T_\lambda\right)^2[\psi_1(\tau)]^{-1}_{\lambda,\lambda'} - [\psi_2(\tau)]_{\lambda,\lambda'}\,, \tag{22}$$

with $[\psi_1(\tau)]^{-1}_{\lambda,\lambda'}$ being the inverse of the matrix

$$[\psi_1(\tau)]_{\lambda,\lambda'} = \delta_{\lambda,\lambda'}(1-n^T_\lambda)n^T_{\lambda'} + n^T_\lambda n^T_{\lambda'}\phi_{\lambda,\lambda'}(\tau), \tag{23}$$

and where $\phi_{\lambda,\lambda'}(\tau) = \sum_k \mathrm{e}^{\tau(\xi_\lambda - \xi_k)} \langle \lambda | k \rangle \langle k | \lambda' \rangle$. The matrix elements of equation (22) also depends on $\psi_2(\tau)$ defined by

$$[\psi_2(\tau)]_{\lambda,\lambda'} = \sum_{\lambda_1} [\psi_1(\tau)]^{-1}_{\lambda,\lambda_1} \left(n^T_{\lambda_1}\right)^2 \phi_{\lambda_1,\lambda}(\tau). \quad (24)$$

The second term in equation (19) depends on $\mathcal{L}^2_{\lambda,\lambda'}(\tau)$ which vanishes at zero temperature and is defined by

$$E_2(\omega) = 2\mathrm{Re}\left\{ \int_0^\infty \mathrm{d}t\ \mathrm{e}^{\mathrm{i}(\omega+\varepsilon_h - \mathrm{i}\eta)t} \times \sum_{kk'} \left[M_k \mathcal{G}^2_{k,k'}(\tau) M^*_{k'} \right] \right\}, \quad (25)$$

where the vertex function, for this case, is given by

$$\mathcal{G}^2_{k,k'}(\tau) = \sum_{\lambda,\lambda'} \mathrm{e}^{\tau\xi_\lambda} n^T_\lambda \langle k | \lambda \rangle \{ \delta_{\lambda,\lambda'} - n^T_{\lambda'} (\phi\mathcal{X})_{\lambda,\lambda'} \} \langle \lambda' | k' \rangle, \quad (26)$$

with

$$(\phi\mathcal{X})_{\lambda,\lambda'} \equiv [\phi\mathcal{X}(\tau)]_{\lambda,\lambda'} = \sum_{\lambda_1} \phi_{\lambda,\lambda_1}(\tau) \mathcal{X}_{\lambda_1,\lambda'}(\tau). \quad (27)$$

The parameter η, in the integrals (20) and (25), is a damping coefficient that guarantees the convergence of the integrals and which along this paper is taken as 0.07 $\hbar\omega_\mathrm{c}$. In order to make the whole numerical processes feasible, such integrals are performed following the procedure detailed in [12] and references therein.

3 Application of the theory

We apply the above theory to the case of an n-doped Q2D system under the presence of both a perpendicular magnetic field B and a weak periodic modulation potential applied in the y-direction of the xy plane. As detailed in reference [19], the modulation potential $V(y) = V_m \cos(Gy)$, where $G = 2\pi/a$, a being the period of the modulation potential. Such a potential can be treated in first order perturbation theory whenever the amplitude of the modulation V_m is small compared with typical energies (cyclotron energies) of the system. Thus, both the energy $\epsilon_{jn}(k)$ and the wavefunction $\psi^1_{nk}(x,y)$ of the electron in a subband jn can be written as

$$\epsilon_{jn}(k) = \varepsilon_j + (n+1/2)\hbar\omega_c + \langle nk | V(y) | nk \rangle, \quad (28)$$

and

$$\psi^1_{nk}(x,y) = \psi^0_{nk}(x,y) + \sum_{n' \neq n} \frac{\psi^0_{n'k}(x,y) \langle n'k | V(y) | nk \rangle}{(n-n')\hbar\omega_c}. \quad (29)$$

Here ω_c is the cyclotron frequency, ε_j is the two-dimensional subband energy in absence of the magnetic field, k is the wave vector in the x-direction, and n is the Landau level index. Also, $\langle n'k | V(y) | nk \rangle$ are matrix elements obtained from

$$\langle x,y | nk \rangle = \psi^0_{nk}(x,y) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{\mathrm{i}kx} \chi_{nk}(y), \quad (30)$$

which is the single-particle wave function in the absence of the modulation potential. Here, $\chi_{nk}(y) = \frac{1}{\sqrt{2^n \pi^{\frac{1}{2}} l_\mathrm{b} n!}} \exp\left[\frac{-(y-y_0)^2}{2l^2_\mathrm{b}}\right] H_n\left(\frac{y-y_0}{l_\mathrm{b}}\right)$, is the harmonic oscillator function in the y-direction, where l_b is the magnetic length, $H_n(x)$ a Hermit polynomial and $y_0 = -l^2_\mathrm{b} k$ is the classical orbit center depending on the wave vector k. We have used the z-direction single-particle wave function as a delta function centered at the origin $z_e = 0$. In our calculations, we will include only one conduction subband, $j = 1$, and two lowest Landau levels, $n = 0, 1$. The subband structure is shown in Figure 3 of reference [19]. Electronic properties of such systems have been extensively studied both theoretically [22,23] and experimentally [14], and we are considering the same single-particle treatment which has been adopted in the theoretical works.

For simplicity, we will use a contact electron-hole interaction of intensity V_h to describe the hole potential at $x = x_h$ and $y = y_h$. Such a potential is defined as

$$V^h_{nk,n'k'} = V_h \psi^1_{nk}(x_h, y_h) \left[\psi^1_{n'k'}(x_h, y_h)\right]^*. \quad (31)$$

As commented before, the optical-created hole is consider as being localized by an impurity, in such a way that (x_h, y_h) is the pair of coordinate localizing it in the plane. Thus, we are working with a dispersionless valence band, *i.e.*, the hole has an infinite mass and can appear with any values of (x_h, y_h). We will assume $x_h = 0$ and study the PL spectra by taking y_h at different positions with respect to the energy of the first Landau level $\epsilon_{n=1}(y_0)$, which is given by

$$\epsilon_{j=1,n=1}(y_0) = \epsilon_{j=1} + 1/2\hbar\omega_c + V_m \mathrm{e}^{(G^2 l^2_\mathrm{b}/4)} \cos(Gy_0). \quad (32)$$

This energy was obtained from equation (28). In absence of the periodic potential, *i.e.* for $V_m = 0$, the Landau level $\epsilon_{j=1,n=1}(y_0)$ is degenerated in y_0. Noticed that when, *e.g.*, $y_h = 0$ the hole is localized just bellow the conduction states at the top of the first Landau level. In the next section we are going to study the effect of different values of y_h on the PL spectra.

3.1 Results for a weak electron-hole interaction

Figure 1 shows finite-temperature emission spectra $E(\omega)$ obtained from the sum of the two terms of equation (19). These results have been calculated for an electron-hole potential strength of $V_{e-h} = -0.03$. The energies are scaled in $\hbar\omega_c$. The parameters used in the calculation are depicted in Figure 3 of reference [19], in which the half occupation of the lowest band is shown ($\nu = 1/2$). The zero

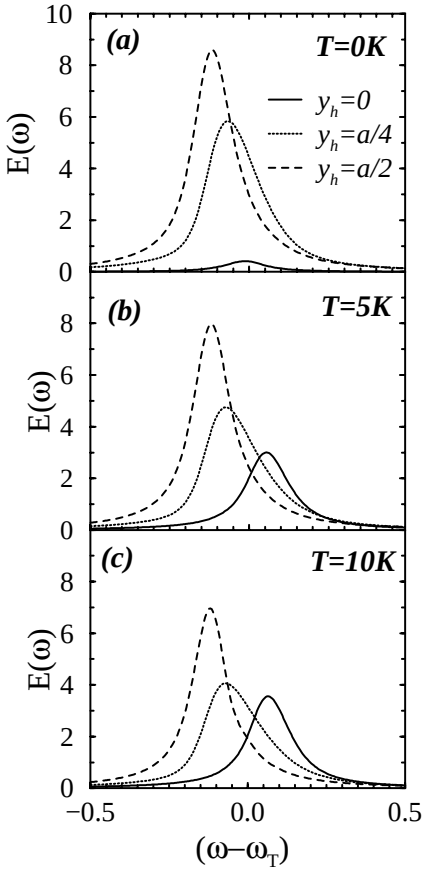

Fig. 1. Finite-temperature PL spectra, $E(\omega)$, for different values of the y-coordinate: $y_h = 0$ (solid lines), $y_h = a/4$ (dot lines) and $y_h = a/2$ (dashed lines). (a) $T = 0$, (b) $T = 5$ K, (c) $T = 10$ K. The strength of the electron-hole contact interaction is taken as -0.03.

for the x-axis, in all PL figures in this paper, is taken as the threshold ω_T, which is defined as the Fermi energy of the system at zero-temperature. We analyze both the zero- and the finite-temperature PL spectra for the cases where the valence hole is localized at three different positions, y_h, with respect to the modulation potential. These positions are depicted by solid lines for $y_h = 0$, dotted lines for $y_h = a/4$ and dashed lines for $y_h = a/2$.

In Figure 1a we show the zero-temperature PL spectra. For $y_h = 0$ (the hole localized just bellow the top of the lowest conduction band), the conduction states are empty at zero temperature. In the absence of the many-body effects (replacement transitions), one would expect that this valence-hole localization should imply a maximum in the PL spectra coming from a direct exciton-like recombination at $(\omega - \omega_T) \simeq 0.12$. This quantity is the energy of the empty states at the top of lowest conduction subband. However, the maximum in the PL spectra, for the $y_h = 0$ case, occurs at an energy bellow the chemical potential, *i.e.* at energy lower than ω_T. Therefore, one deduces that, in the $y_h = 0$ situation, the replacement transitions originated by occupied states, are responsible by the blueshift of the peak to energies below the Fermi energy. Such a kind of behavior of the PL is a characteristic effect of a FES.

On the other hand, for $y_h = a/4$, the hole is localized just bellow the conduction states at the vicinity of the Fermi level for the $\nu = 1/2$ situation. The blueshift related to the replacement transitions also occurs since one would expect that, in the absence of the many-particle effects, the maximum of the PL spectra would occur at the energy of the conduction band states in the vicinity the Fermi level, *i.e.* at an energy $(\omega - \omega_T) \simeq 0$. Moreover, since in the $y_h = a/4$ case the hole is localized spatially closer to the occupied conduction states, our results show that the peak of $y_h = a/4$ curve is more intense than that of the $y_h = 0$ case, as one would expect.

In the case where the hole has suddenly appeared at $y_h = a/2$ position, *i.e.* just bellow the states at the bottom of the lowest conduction band, we observe the largest intensity in the PL spectra. In this case the blueshift appearing in previous cases, does not occur since the maximum of the $y_h = a/2$ curve is located at the energy of the occupied states corresponding to the bottom of the lowest conduction subband at $(\omega - \omega_T) \simeq -0.12$. The absence of any blueshift of the PL spectrum makes difficult to identify the many-body effects.

Some important conclusions are drawn from Figure 1a. The first one is to observe that, as one moves the hole from $y_h = a/2$ to $y_h = 0$, the density of occupied states can be naturally mapped out. The second conclusion is that the most remarkable many-body effect occur when the hole is localized just bellow the empty conduction states in the vicinity of the Fermi sea. This case is achieved when the hole is localized at the positions between $y_h = 0$ and $y_h = a/4$.

Figures 1b and 1c show the temperature dependence of the PL curves given in Figure 1a. For $y_h = a/2$ and $y_h = a/4$, there is a decrease of the intensity of the PL peaks as the temperature increases. The effect of the temperature on the PL spectra, for these two cases, is similar to those observed on the FES [24]. On the other hand, the temperature variation of the PL spectra for $y_h = 0$, shows both a significantly intensity increase and a redshift of the PL peak for increasing temperature. These effects on the $y_h = 0$ curve occur because the temperature populates the electronic states in the vicinity the Fermi level so that, they contribute to the PL process. According to the finite-temperature results shown in Figure 1, one can also observe that the cases which depend strongly on the temperature variation are those in which the valence hole is localized just bellow the empty conduction states, in the vicinity of the Fermi surface at $y_h = 0$ and $y_h = a/4$ cases. This is due to the fact that the FES depends on the behavior of the vicinity the Fermi surface whose empty states will give rise to the electron-hole pairs region which will appear for temperatures different from zero.

Since our main goal is to discriminate the importance of the new term $\mathcal{L}^2_{\lambda,\lambda'}(\tau)$ presented in Section 2 , we show in Figure 2, the part of the PL spectrum produced by $E_1(\omega)$. The difference between Figures 1 and 2 is due to replacement transitions characterized by $E_2(\omega)$.

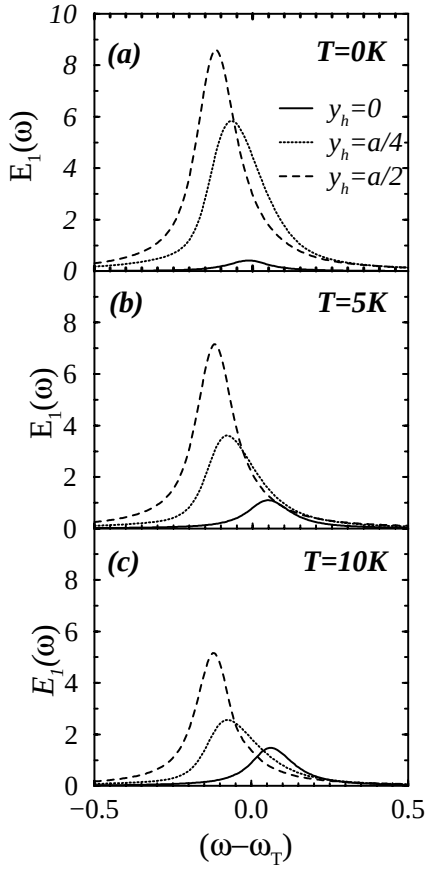

Fig. 2. Part of the finite-temperature PL spectra represented by the transitions characterized by the term $E_1(\omega)$. Different values of the y-coordinate are also show: $y_h = 0$ (solid lines), $y_h = a/4$ (dot lines) and $y_h = a/2$ (dashed lines). (a) $T = 0$, (b) $T = 5$ K, (c) $T = 10$ K. The strength of the electron-hole contact interaction is the same of Figure 1.

As discussed in Section 2, $E_2(\omega)$ represents the transitions mediated by exchange processes provided by those occupied states which belong to the thermally excited electron-hole pair region. This kind of transitions do not exist at zero temperature so that, Figures 1a and 2a are identical. By analyzing the finite-temperature results presented in Figures 1 and 2 one can see that the effect of the $E_2(\omega)$ on the PL spectra is to provide the evidence of the FES and causing an increase in all the peaks for different values of y_h. Finally, we would like to stress that the transitions represented by $E_2(\omega)$ have important contributions to the total intensity of the PL spectra.

3.2 Results for a strong electron-hole interaction

In this subsection we will discuss the effect of the electron-hole-interaction enhancement on the PL spectra. We are going to analyze PL spectra where the strength of the electron-hole potential V_{e-h} is taken as -0.08.

First, we are going to analyze the finite-temperature PL spectra of the $\nu = 1$ regime of the QHE. Our goal here is to investigate both the temperature and the many-body effects on such a regime. The many-body effect is responsible by the shake-up processes of the Fermi sea, as the emission of a photon takes place, and leading to a rearrangement of the final single-particle states to a new situation without the presence of the valence hole. This type of shake-up process is characterized by the existence of an electron-hole pair in the final many-body state. The electron-hole pair creation is an exclusive consequence of the photon emission process and, therefore, it may occur even at zero temperature.

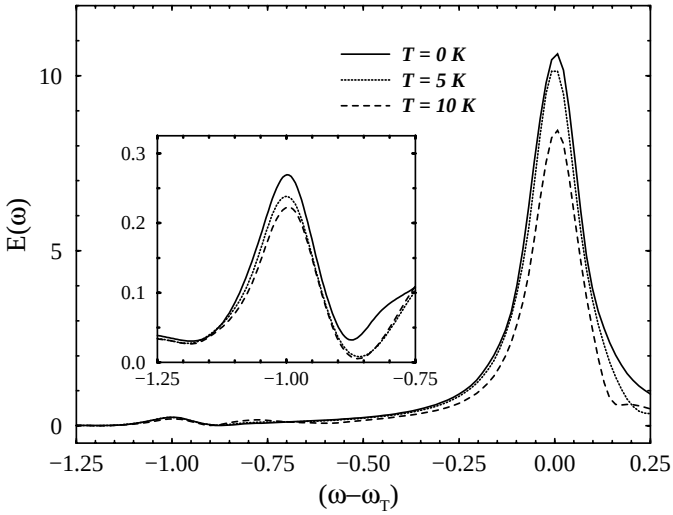

Fig. 3. Total PL spectra, $E(\omega)$ at $\nu = 1$ ($V_m = 0$). Inset shows the temperature dependence of the shake-up structure.

By increasing the strength of V_{e-h} to -0.1, we present, in Figure 3, the finite-temperature PL spectra given by $E(\omega)$ for $\nu = 1$ quantum Hall regime (without spin). This regime has been achieved, in our calculation, by taking a very weak modulation potential V_m, *i.e.* $V_m \simeq 0$. In this situation, the lowest conduction subband becomes dispersionless and fully occupied ($\nu = 1$). Figure 3 shows the temperature dependence of the main peak, at $(\omega - \omega_T) \simeq 0$, and corresponding to those recombinations from the lowest Landau level. A shake-up structure appears clearly at $(\omega - \omega_T) \simeq -1$. The difference between the energy position of the main transition peak and the shake-up structure is associated to the energy of the electron-hole pair which appears in the many-body final state. A very important point to be stressed is that, in our calculation, shake-up structures are possible because $V_{e-e} \neq -V_{e-h}$. Therefore, no hidden symmetry [25] exists and many-body effects can be observed in PL at $\nu \leq 1$. The inset of Figure 3 shows how the intensity of the shake-up structure decreases with the temperature. One can interpret such an intensity decrease as follows: the creation of the final electron-hole pair becomes a less likely process since the temperature tends to populate the empty states in the second-Landau-band which will give rise to the final electron-hole pair. The shake-up structure has not been completely destroyed because at this value of temperature, thermal excitation is not able to populate those empty states in the second Landau level ($T = 10$ K $\rightarrow 0.148\ \hbar\omega_c$).

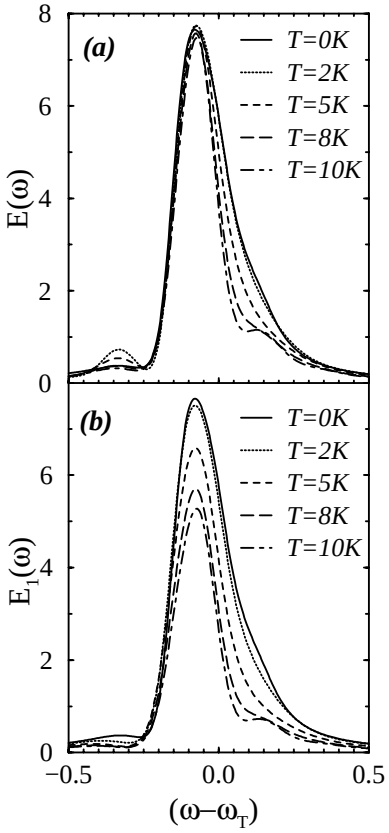

Fig. 4. Finite-temperature PL spectra for the case in which the hole is located in $y_h = a/4$ and for some values of temperature. (a) Total PL spectra, $E(\omega)$. (b) Part of the finite-temperature PL spectra represented by the term $E_1(\omega)$.

Let us return to the case in which V_m is taken as 0.15 and V_{e-h} is given by -0.08. This situation is characterized by the filling factor $\nu = 1/2$.

We show in Figure 4a, the effects of temperature for the $y_h = a/4$ case. As the electron-hole interaction increases, our finite-temperature results show the development of a small structure in the low energy region around $(\omega - \omega_T) \simeq -0.30$. This structure already present at $T = 0$, reaches a maximum height for a given range of temperature. For further increase of the temperature, those unoccupied states at the lowest conduction subband become populated, which leads to a decrease of the intensity of this structure. For temperatures larger than $T = 10$ K this structure practically disappears, showing that those empty conduction states are responsible for the appearance of this structure. As the structure at the low energy side of the main peak becomes smaller, we can also see that conduction states thermally populated contribute to the PL spectrum, producing a small shoulder on the high energy side of the main peak, around $(\omega - \omega_T) \simeq 0.12$.

The small structure in the low energy side of the main peak, can be interpreted as follows: it corresponds to shake-up processes of the Fermi sea, as the emission of a photon takes place leading to a rearrangement of the final single-particle states to a new situation without the presence of the valence hole. As mentioned above, this shake-up process is characterized by the existence of an electron-hole pair in the final many-body state. Notice that when temperature increases and the unoccupied states at the lowest conduction subband become more and more populated, the creation of such a final electron-hole pair becomes a less likely process, once there will be less empty states available in lowest conduction subband.

We would like to comment on eventual self-energy effects on the shake-up results. The rate of making an electron hole pair in the final state of the system, called as $R(\omega)$ [9], quantifies the hole self-energy effects, which should contribute to the intensity of the shake-ups once included in the calculation. However, it would not result in the appearance of different shake-up structures; it would only contribute to the intensity of those structures which would come from the electronic part of the correlation function. The electronic part of the correlation function, by itself, already shows shake-up structures.

Furthermore, as pointed out before, we have neglected the electron-electron (e-e) scattering and assumed an infinitely long quasiparticle lifetime. Actually, this lifetime should become shorter as the temperature increases since the (e-e) scattering plays an important role. Such a scattering can be taken into account by including the *electron* self-energy, which can be obtained within the GW approximation. Such a self-energy becomes important at the Fermi surface when the temperature increases [26]. However, the (e-e) scattering can be neglected in this work since we are working with small values of temperature. Finally, we would like to stress that the main purpose here is to investigate the new temperature contributions coming from the electronic part of the PL correlation function. The inclusion of effects such as the electron-electron and hole-hole scattering, is the subject of a future interest.

In order to verify the finite-temperature contribution of the term $E_2(\omega)$ to the total PL spectra, we show in Figure 4b the PL spectrum calculated with the term $E_1(\omega)$ only. One can see the effect of the replacement transitions, represented by $E_2(\omega)$, by analyzing the difference between the curves of Figures 4a and 4b. Observe that the term $E_2(\omega)$, on top of causing a strong enhancement in the intensity of the main peak, also represents a finite-temperature contribution to the increased intensity of the shake-up structure. On the other hand, the small structure appearing in the $T = 0$ curve is quickly destroyed at a very small finite temperature. This means that the term $E_1(\omega)$ presents a small finite-temperature contribution to the shake-up. Therefore, replacement transitions give the main contribution to the shake-up processes in systems with modulated Landau levels.

4 Conclusions

In conclusion the addition of the temperature effects on the MND current-current correlation function which describes the PL spectra of doped semiconductors was reported. We have found new terms arising from the nonunitarity property of the projection-like operator. We have

applied this finite-temperature approach to study temperature and many-body effects on the PL Fermi-edge spectra of a Q2D system under both a perpendicular magnetic field and a weak periodic modulation potential. We have studied the effect of the electron-hole interaction strength on the spectra. There are Fermi sea shake-up processes, whose temperature behavior and dependence on the valence hole position, have been thoroughly analyzed.

The finite-temperature approach presented in this paper provide an important tool towards the understand of the behavior of FES intensities as a function of the temperature. This behavior depends on the effects which are determined by the new finite-temperature terms of the PL correlation function. Although the direct comparison with the experimental results should require a better description of the valence-hole, the experimental study of a Q2D system as the one discussed theoretically in this paper, can confirm the importance of the new finite-temperature term of the PL correlation function.

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References

1. *Optical Phenomena in Semiconductor Structures of Reduced Dimensions*, edited by D.J. Lockwood, A. Pinczuk NATO ASI Series E, Vol. 248 (Kluwer Academic Publishers, Dordrecht, 1993).
2. K. Asano, T. Ando, in *Proceedings of the EP2DS (Electronic properties of two-dimensional Systems)*, 1997, p. 233; G. Finkelstein, H. Shtrikman, I. Bar-Joseph, *ibid.*, p. 237; J.I. Osborn, A.J. Shields, M.Y. Simmons, N.R. Cooper, D.A. Ritchie, M. Pepper, *ibid.*, p. 241; M. Potemski, L. Gravier, A. Trüby, D.K. Maude, P. Hawrylak, Zb. Wasilewski, B. Etienne, *ibid.*, p. 553; R.J. Nicholas, D. Kinder, A.N. Priest, C.C. Chang, H.H. Cheng, J.J. Harris, C.T. Foxon, *ibid.*, p. 557; H.D.M. Davies, J.C. Harris, R.L. Brockbank, J.F. Ryan, A.J. Turberfield, M.Y. Simmons, D.A. Ritchie, *ibid.*, p. 709; F. Plentz, D. Heiman, A. Pinczuk, L.N. Pfeiffer, K.W. West, *ibid.*, p. 863.
3. S.E. Barret, G. Dabbagh, L.N. Pfeiffer, K.W. West, R. Tycho, Phys. Rev. Lett. **74**, 5112 (1995).
4. G. Finkelstein, H. Shtrikman, I. Bar-Joseph, Phys. Rev. B **56**, 10326 (1997).
5. H.P. van der Meulen, J. Rubio, J.M. Calleja, C. Tejedor, F. Rodriguez, V. Haerle, F. Scholz, in *Proceedings of the EP2DS (Electronic properties of two-dimensional Systems)*, 1997, p. 847.
6. N.R. Cooper, D.B. Chklovskii, Phys. Rev. B **55**, 2436 (1997).
7. K. Ohtaka, Y. Tanabe, Rev. Mod. Phys. **62**, 929 (1990).
8. T. Uenoyama, L.J. Sham, Phys. Rev. Lett. **65,** 1048 (1990).
9. G.D. Mahan, *Many-Particle Physics* (Plenum, New York, 1981).
10. P. Nozières, C.T. De Dominicis, Phys. Rev. **178,** 1097 (1969).
11. G.D. Mahan, Phys. Rev. B **21,** 1421 (1980).
12. P. Hawrylak, Phys. Rev. B **44,** 3821 (1991).
13. P. Hawrylak, Phys. Rev. B **44**, 3821; 6262; 11236 (1991).
14. J.M. Calleja, A.R. Goñi, A. Pinczuk, B.S. Dennis, J.S. Weiner, L.N. Pfeiffer, K.W. West, Phys. Rev. B **51**, 4285 (1995).
15. M.S. Skolnick, J.M. Rorison, K.J. Nash, D.J. Mowbray, P.R. Tapster, S.J. Bass, A.D. Pitt, Phys. Rev. Lett. **58**, 2130 (1987); I.V. Kukushkin, K.V. Klitzing, K. Ploog, V.E. Kirpichev, B.N. Shepel, Phys. Rev. B **40**, 4179 (1990).
16. A.S. Plaut, H. Lage, P. Grambow, D. Heitmann, K. von Klitzing, K. Ploog, Phys. Rev. Lett. **67** 1642 (1991).
17. M. Combescot, P. Nozières, J. Phys. France **32**, 913 (1971).
18. M. Tavares, C. Tejedor, Surf. Sci. **361**; **362**, 788 (1996).
19. M. Tavares, C. Tejedor, G.E. Marques, Phys. Rev. B **56**, 9753 (1997).
20. J. Friedel, Comments Solid State Phys. **2**, 21 (1969).
21. R.R. Gerhardts, D. Weiss, K.V. Klitzing, Phys. Rev. Lett. **62**, 1173 (1989).
22. U. Wulf, V. Gudmundsen, R.R. Gerhardts, Phys. Rev. B **28**, 4218 (1988), and references therein.
23. A.K. Geim, R. Taboryski, A. Kristensen, S.V. Dubonos,, P.E. Lindelof, Phys. Rev. B **46**, 4324 (1992); A. Manolescu, R.R. Gerhardts, Phys. Rev. B **51**, 1703 (1995); S.M. Stewart, C. Zhang, Phys. Rev. B **52**, R17036 (1995); Q.W. Shi, K.Y. Szeto, Phys. Rev. B **53**, 12990 (1996).
24. F.J. Rodriguez, C. Tejedor, Phys. Rev. B **47,** 1506 (1993); *ibid.,* 13015; Phys. Rev. B **49,** 16781 (1994).
25. A.H. MacDonald, E.H. Rezayi, Phys. Rev. B **42**, 3224 (1990); A.H. MacDonald, E.H. Rezayi, D. Keller, Phys. Rev. Lett. **68**, 1939 (1992).
26. M. Tavares, G.-Q. Hai, (unpublished).