Coulomb Energy of a Quasi-2D Electron Gas in a Quantum Well

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(Received 19 January 1994)

We calculate the Hartree, exchange and correlation energies of a quasi-2D electron gas in doped semiconductor quantum wells, using an expansion in Coulomb interaction. This expansion, also valid for the Hartree term in usual experimental situations, allows one to obtain the analytical well width dependence of the energies. We find that the finite width corrections to the exact 2D exchange-correlation energy are quite often as large as the Hartree contributions.

PACS numbers: 73.20.Dx

In the past decade, a large amount of work has been devoted to the study of quasi-two-dimensional electron gas appearing in semiconductor quantum wells, multiple quantum wells, and superlattices. Many-body effects in these quasi-2D systems are usually investigated *via* the local density approximation [1–7]. In this formalism, the Hartree energy is calculated exactly through the self-consistent resolution of coupled Schrödinger-Poisson equations, while the exchange-correlation contribution is treated in an approximate way: The corresponding many-body effects which are inherently nonlocal, are included as a one particle potential which depends on the local value of the density only. It is usually considered valid only for density variations small on the scale of the Wigner-Seitz radius [1, 8], a condition obviously violated in quantum wells. For these structures, another treatment of many-body effects is thus necessary [8–12].

In this Letter, we present a new approach to the quasi-2D electron gas energy, in which the exchange-correlation contribution is treated in the same way as the Hartree part. It is based on a perturbative treatment [13, 14] of the Coulomb interaction similar to the one used for 3D and exact 2D electron gases. This approach, which has been shown to be very accurate for the Hartree energy [15] in usual cases (electrons in the lowest subband only and well width smaller than the Bohr radius), allows a very standard calculation of the exchange-correlation energy and has the advantage of giving the analytical well width dependence of all terms. We find that the finite width corrections to the exact 2D exchange-correlation energy are quite often as large as the Hartree energy, which means that these two contributions must be placed on the same footing.

A finite well width induces two kinds of effects when compared to the exact 2D limit: (i) the usual Coulomb interaction (associated with finite momentum transfer processes) depends on the well width *via* a form factor; and (ii) new zero momentum transfer processes appear, which give rise to the Hartree energy [15], and also play a role in the exchange-correlation terms, due to mixed $\mathbf{q} \neq \mathbf{0}$ and $\mathbf{q} = \mathbf{0}$ processes.

The physics of quasi-2D electron gas is controlled by two dimensionless parameters, r_s and λ. The first one is related to the 2D electron density $n_s = N/S = K^2/2\pi$, through the relation $n_s \pi r_s^2 a_0^2 = 1$, $a_0 = \hbar^2/me^2$ being the Bohr radius. The other parameter is related to the well width and can be taken [16] as $\lambda = (2\pi)^{-1} Ka$. A Coulomb expansion of the energy implies, as usual, $r_s < 1$. For electrons in the lowest subband only ($\varepsilon_1 + \varepsilon_K < \varepsilon_2$ with $\varepsilon_K = \hbar^2 K^2/2m$ and $\varepsilon_n = n^2\hbar^2\pi^2/2ma^2$), we have $\lambda < \lambda_0 = \sqrt{3}/2$, i.e., $a/a_0 < \pi\sqrt{3/2}r_s$. A Coulomb expansion of the energy for electrons in the lowest subband thus corresponds to $0.26a/a_0 < r_s < 1$ (this restricts the well width to be at most of the order of the Bohr radius). Note that a perturbative expansion of the energy could be performed for smaller r_s, i.e., for electrons in more than one subband. However, this raises new problems which are beyond the scope of this Letter.

Let us consider a system composed of electrons confined in a well with infinitely high barriers, and ions with density $n_s\rho_i(z)$ located inside or outside the electron layer. The total electron-electron, ion-ion, and electron-ion interaction can be split into two parts corresponding to excitations with zero and nonzero momentum transfers. The first part, which induces the Hartree processes, reads [15] in terms of $a^\dagger_{nk\sigma}$ creation operators for free electrons in the nth subband

$$V^{q=0} = \frac{1}{2}\,\frac{2\pi e^2}{Sa^{-1}} \sum_{\substack{n_1 n_1' n_2 n_2' \\ \mathbf{k}_1\mathbf{k}_2\sigma_1\sigma_2}} W_{n_1 n_1';n_2 n_2'} a^\dagger_{n_1\mathbf{k}_1\sigma_1} a^\dagger_{n_2\mathbf{k}_2\sigma_2} a_{n_2'\mathbf{k}_2\sigma_2} a_{n_1'\mathbf{k}_1\sigma_1}\,, \tag{1}$$

$$W_{n_1 n_1';n_2 n_2'} = -\int\int dz_1\, dz_2 \frac{|z_1 - z_2|}{a} [\varphi^*_{n_1}(z_1)\varphi_{n_1'}(z_1) - \rho_i(z_1)\delta_{n_1 n_1'}][\varphi^*_{n_2}(z_2)\varphi_{n_2'}(z_2) - \rho_i(z_2)\delta_{n_2 n_2'}],$$

where $\varphi_n(z) = (2/a)^{1/2}\sin(n\pi z/a)$ for $0 \le z \le a$. The diagonal terms $W_{nn;n'n'}$ depend essentially on the electron-ion separation and are large for electrons and ions far apart. The other terms depend on the ion configuration only (ions located inside, on one side or on both sides of the electron layer).

The Coulomb interaction with nonzero momentum transfers reads

$$V^{q\neq 0} = \frac{1}{2}\sum_{\mathbf{q}\neq 0}\frac{2\pi e^2}{Sq}\sum_{\substack{n_1n_1'n_2n_2'\\ \mathbf{k}_1\mathbf{k}_2\sigma_1\sigma_2}} V_{n_1n_1';n_2n_2'}(aq/2\pi)a^{\dagger}_{n_1\mathbf{k}_1+\mathbf{q}\sigma_1}a^{\dagger}_{n_2\mathbf{k}_2-\mathbf{q}\sigma_2}a_{n_2'\mathbf{k}_2\sigma_2}a_{n_1'\mathbf{k}_1\sigma_1}\,,$$

$$V_{n_1n_1';n_2n_2'}(Q) = \int\int dz_1\,dz_2\exp[-2\pi Q\,|z_1 - z_2|/a]\varphi^*_{n_1}(z_1)\varphi_{n_1'}(z_1)\varphi^*_{n_2}(z_2)\varphi_{n_2'}(z_2)\,. \tag{2}$$

The form factor $V_{n_1n_1';n_2n_2'}(0)$ reduces to $\delta_{n_1n_1'}\delta_{n_2n_2'}$ while for small Q, its nondiagonal part vanishes as Q.

The quasi-2D electron gas Coulomb energy is obtained as a perturbative expansion in $V_{\mathrm{Coul}} = V^{q\neq 0} + V^{q=0}$, generating terms in $[V^{q\neq 0}]^n[V^{q=0}]^p$. The Hartree energy corresponds to all terms with $n = 0$ and $p \ge 1$. By analogy with the exact 2D case, we call "exchange energy" the sum of terms with $n = 1$ and $p \ge 0$, the correlation energy including all the other terms ($n \ge 2$ and $p \ge 0$). We now calculate the main contributions to these energies in the small r_s limit, in order to assess their relative importance.

(1) The *Hartree energy* which results from charge separation is controlled [15,16] by a dimensionless parameter which must vanish with a, n_s, and e^2, namely $\lambda_H = K^2a^3/\pi^4a_0 = (4\sqrt{2}/\pi)\,r_s\lambda^3$. Its Coulomb expansion thus appears as a small λ_H expansion. The two lowest order terms [diagrams (H_1) and (H_2) of Fig. 1] read

$$E_H = \langle 0|V^{q=0}|0\rangle + \sum_{M\neq 0}|\langle M|V^{q=0}|0\rangle|^2/(E_0 - E_M)$$

$$= NR_0[a_Hr_s\lambda^3 - b_H(r_s\lambda^3)^2 + O(r_s\lambda^3)^3]/r_s^2\lambda^2, \tag{3}$$

where $R_0 = me^4/2\hbar^2$ is the Rydberg. A part of a_H depends on the electron-ion distance and corresponds to the electrostatic energy necessary to separate electrons from ions. The other part, as well as b_H, depends on the ion configuration, and is associated with the deformation of the electron distribution in the electron-ion field. These coefficients are given in Table I, for three typical ion configurations: The "in" case corresponds to ions uniformly distributed inside the electron layer, the "out 1" and "out 2" cases to ions uniformly distributed in *one* or *two* adjacent layers of width a or $a/2$.

Note that for electrons in the lowest subband only ($\lambda_H \le 0.3a/a_0$), the λ_H^3 term of E_H [diagrams (H_3) and (H_3')] is very small for usual well widths ($a \lesssim a_0$).

(2) The *exchange energy* contains all terms in $V^{q\neq 0}[V^{q=0}]^p$ with $p \ge 0$. Its small r_s leading term [14] [diagram (X_0)] reads

$$E_{X_0} = \langle 0|V^{q\neq 0}|0\rangle = -NR_0r_s^{-1}A_X(\lambda), \tag{4}$$

$$A_X(\lambda) = \frac{1}{\sqrt{2}\pi^2}\int_{Q_1<1}\int_{Q_2<1} d^2Q_1\,d^2Q_2\,\frac{V_{11;11}(\lambda|\mathbf{Q}_1 - \mathbf{Q}_2|)}{|\mathbf{Q}_1 - \mathbf{Q}_2|}\,.$$

For electrons in the lowest subband, $A_X(\lambda)$ decreases from the exact 2D result [17] $A_X(0) = 8\sqrt{2}/3\pi = 1.200$ to $A_X(\lambda_0) = 0.750$.

The next term [diagram (X_1)] is a mixed Hartree-exchange term:

$$E_{X_1} = \sum_{M\neq 0}[\langle 0|V^{q=0}|M\rangle\langle M|V^{q\neq 0}|0\rangle + \text{c.c.}]/(E_0 - E_M) = NR_0\lambda^4B_X(\lambda),$$

$$B_X(\lambda) = \frac{32}{\pi}\sum_{n>1}\frac{W_{11;1n}}{n^2-1}\int_{Q_1<1}\int_{Q_2<1} d^2Q_1\,d^2Q_2\,\frac{V_{11;1n}(\lambda|\mathbf{Q}_1-\mathbf{Q}_2|)}{\lambda|\mathbf{Q}_1-\mathbf{Q}_2|}\,. \tag{5}$$

$B_X(\lambda)$ is a decreasing function of λ which depends on the ion configuration *via* $W_{11;1n}$ (see Table I).

Exchange contributions with two $V^{q=0}$ [diagrams (X_2), (X_2'), (X_2'')] are in r_s. For small λ's, the dominant one is in $NR_0r_s\lambda^6$.

The total exchange energy thus reads

$$E_X/NR_0 = -r_s^{-1}A_X(\lambda) + \lambda^4B_X(\lambda) + O(r_s)\,. \tag{6}$$

(3) In the small r_s limit, the leading contribution to the *correlation energy* contains two $V^{q\neq 0}$ only and is similar to the second term of Eq. (3). We can divide it into two terms, "normal" and "anomalous."

The normal term [diagrams $(C^d_{0,2})$ and $(C^e_{0,2})$] corresponds to the usual direct and exchange second order correlation terms, with possible intersubband transitions due to the Coulomb form factor:

$$E^{d+e}_{C_{0,2}} = \left(\frac{2\pi e^2}{S}\right)^2 \sum_{\mathbf{q}\neq 0} \sum_{\substack{n_1 n_2 \\ \mathbf{k}_1 \mathbf{k}_2}} \left[\frac{2V^2_{1n_1;1n_2}(\lambda q/K)}{q^2} - \frac{V_{1n_1;1n_2}(\lambda q/K) V_{1n_1;1n_2}(\lambda|\mathbf{q}+\mathbf{k}_1-\mathbf{k}_2|/K)}{q|\mathbf{q}+\mathbf{k}_1-\mathbf{k}_2|} \right] \times \frac{f_{\mathbf{k}_1}(1-\delta_{1n_1} f_{\mathbf{k}_1+\mathbf{q}}) f_{\mathbf{k}_2}(1-\delta_{1n_2} f_{\mathbf{k}_2-\mathbf{q}})}{2\varepsilon_1 - \varepsilon_{n_1} - \varepsilon_{n_2} + \varepsilon_{\mathbf{k}_1} + \varepsilon_{\mathbf{k}_2} - \varepsilon_{\mathbf{k}_1+\mathbf{q}} - \varepsilon_{\mathbf{k}_2-\mathbf{q}}}$$

$$= -NR_0[B_c^{\text{intra}}(\lambda) + \lambda^2 B_c^{\text{inter}}(\lambda)], \tag{7}$$

where $f_{\mathbf{k}} = \theta(K-k)$, is the step function. The intrasubband contribution ($n_1 = n_2 = 1$) decreases from $B_c^{\text{intra}}(0) = 0.385$ [18–20] to $B_c^{\text{intra}}(\lambda_0) = 0.124$, while $B_c^{\text{inter}}(\lambda)$ is nearly constant (~ 0.04 for $0 < \lambda < \lambda_0$), so that the intersubband contribution increases as λ^2, but remains very small when compared to the intrasubband term.

The anomalous term [diagrams $(C^a_{0,2})$] does not exist in the exact 2D limit [21]. It also results from intersubband processes and reads

$$E^a_{C_{0,2}} = 2\left(\frac{2\pi e^2}{S}\right)^2 \sum_{\substack{n>1 \\ \mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}} \frac{f_{\mathbf{k}_1} f_{\mathbf{k}_2} f_{\mathbf{k}_3}}{\varepsilon_1 - \varepsilon_n} \frac{V_{11;1n}(\lambda|\mathbf{k}_3-\mathbf{k}_1|/K) V_{11;1n}(\lambda|\mathbf{k}_3-\mathbf{k}_2|/K)}{|\mathbf{k}_3-\mathbf{k}_1||\mathbf{k}_3-\mathbf{k}_2|}$$

$$= -NR_0\lambda^4 B_c^a(\lambda). \tag{8}$$

$B_c^a(\lambda)$ decreases from $B_c^a(0) = 0.080$ to $B_c^a(\lambda_0) = 0.009$.

The terms with two $V^{q\neq 0}$ and one $V^{q=0}$ [like diagram $(C^d_{1,2})$] give a contribution in r_s which is of the order of $NR_0 r_s \lambda^4$ for small λ's. These terms have to be compared to terms with three $V^{q\neq 0}$, which are *a priori* of the same order in r_s. Among them, the term corresponding to diagram $(C^d_{0,3})$ is singular in the small q limit. Its singularity, removed by summing up all "ring" diagrams, leads [18, 19] to a contribution of the order of $NR_0 r_s \ln r_s$ instead of $NR_0 r_s$, as obtained from other (regular) terms with three $V^{q\neq 0}$ [like diagram $(C^m_{0,3})$].

We thus find for the correlation energy leading terms

$$E_C/NR_0 = -[B_c^{\text{intra}}(\lambda) + \lambda^2 B_c^{\text{inter}}(\lambda) + \lambda^4 B_c^a(\lambda)] + O(r_s \ln r_s). \tag{9}$$

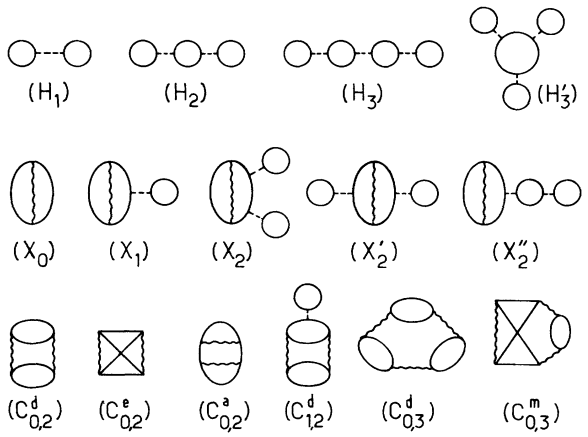

FIG. 1. Hartree (H_p), exchange (X_p), and direct $(C^d_{p,n})$, exchange $(C^e_{p,n})$, anomalous $(C^a_{p,n})$ correlation diagrams with respectively zero, one, and n finite-momentum transfer interactions (wavy lines) and p zero-momentum transfer interactions (dotted lines). The $(C^m_{0,3})$ diagram is a mixed direct-exchange correlation diagram.

(4) From the above results, the *Coulomb energy of a quasi-2D electron gas* can be written as

$$E_H + E_X + E_C = NR_0\{r_s^{-1}[-1.200 + A(\lambda)] + [-0.385 + B(\lambda)] + O(r_s \ln r_s)\}. \tag{10}$$

$A(\lambda)$ and $B(\lambda)$, shown in Fig. 2, are the corrections induced by the finite well width to the first two terms of the exact 2D energy. We now discuss the relative importance of the various contributions to $A(\lambda)$ and $B(\lambda)$, and make a few remarks on the discarded terms.

$A(\lambda)$, defined as

$$A(\lambda) = a_H\lambda + [A_X(0) - A_X(\lambda)], \tag{11}$$

comes from Hartree and exchange first order terms. Its largest contribution comes from the electrostatic energy necessary to separate ions from electrons when the ions lie outside the electron layer. The other Hartree contribution, due to the deformation of the electron distribution, is of the order of the well width effect on the exchange energy.

$B(\lambda)$, defined as

$$B(\lambda) = \Delta B_c^{\text{intra}}(\lambda) - \lambda^2 B_c^{\text{inter}}(\lambda) - \lambda^4[b_H - B_X(\lambda) + B_c^a(\lambda)] \tag{12}$$

TABLE I. Hartree coefficients a_H and b_H [cf. Eq. (3)] and mixed Hartree-exchange coefficient $B_X(\lambda)$ [cf. Eq. (5)] for three different ion configurations (see text).

Ion Configuration	a_H	b_H	$B_X(0)$	$B_X(\lambda_0)$
"in"	0.225	0.051	0.127	0.043
"out 2"	4.087	0.318	0.318	0.107
"out 1"	12.973	7.159	0.318	0.107

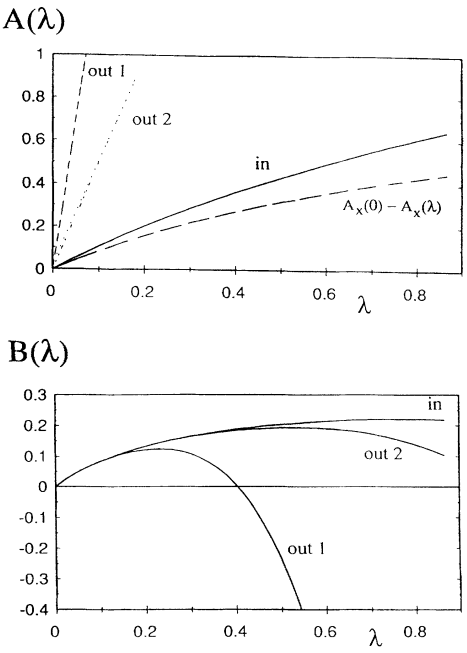

FIG. 2. $A(\lambda)$ and $B(\lambda)$ are the corrections to the exact 2D values of the first and second order Coulomb energy terms. "in," "out 2," and "out 1" correspond to different ion configurations (see text). The λ dependence of the exchange first order term $A_X(\lambda)$ is also shown. In the "out" cases, $A(\lambda)$ is dominated by a mere electrostatic Hartree term so that it varies almost linearly. $B(\lambda)$ is dominated by the correlation term for small λ's and by the Hartree term for large λ's in the "out 1" case only.

with $\Delta B_c^{\text{intra}}(\lambda) = B_c^{\text{intra}}(0) - B_c^{\text{intra}}(\lambda)$, comes from the Hartree second order term, the mixed Hartree-exchange term, and the second order correlation term composed of intrasubband and intersubband direct and exchange contributions plus the anomalous contribution.

For small λ's, $B(\lambda)$ is dominated by the intrasubband direct and exchange correlation term $\Delta B_c^{\text{intra}}(\lambda)$. For $\lambda \approx \lambda_0$, this is still true when the ions are *inside* the electron layer. When the ions are *outside*, the $\lambda_0^4 B_X(\lambda_0)$ Hartree-exchange term is roughly $0.2\Delta B_c^{\text{intra}}(\lambda_0)$. As for the second order Hartree term, it is dominant when the ions are all on one side of the electron layer, while it is of the order of $\Delta B_c^{\text{intra}}(\lambda_0)$ when the ions are on both sides.

The next term, in $r_s \ln r_s$, comes from the third order "ring" diagram, screened by higher order ring contributions. All other third order terms are in r_s. Among them, the Hartree and mixed Hartree-exchange third order terms are completely negligible even for intermediate λ's since they are in $r_s\lambda^7$ and $r_s\lambda^6$, respectively.

In conclusion, we have calculated the Hartree, exchange and correlation energies of a quasi-2D electron gas as an expansion in Coulomb interaction. We have shown that, besides a mere electrostatic term which can be large when the electron-ion distance is large, the Hartree energy is smaller than or of the order of the well width corrections to the exact 2D exchange and correlation terms (except when ions are all on one side of the electron layer *and* the electron filling approaches the $n = 2$ subband). Consequently, it is inconsistent to include the Hartree second order term, or to calculate the Hartree energy self-consistently as in the local density approximation, without taking accurately into account the well width effect on the exchange-correlation terms.

We wish to thank C. Benoit à la Guillaume and J. Y. Vinet for useful discussions. Groupe de Physique des Solides is CNRS URA 17.

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