Exchange effects in a quasi-one-dimensional electron gas

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We calculate the electron exchange of a quasi-one-dimensional electron gas in a quantum-well wire of radius R_0. A two-subband model is considered and the exchange self-energy for the first and second subband is calculated under the assumption that only the lowest subband is partially filled with electrons. Band-bending effects are also discussed. Results for the total energy per electron including kinetic and exchange energy are presented.

I. INTRODUCTION

The subband structure of quasi-one-dimensional electron systems (Q1D ES) as realized in quasi-one-dimensional quantum wires is presently under study in experiments (for a review, see Ref. 1) and in theory (for a review, see Ref. 2). In realistic calculations of the subband structure only numerical results are available[3] which neglect many-body effects.

Many-body effects are known to enlarge the intersubband spacing in two-dimensional systems (for a review, see Ref. 4). Exchange effects have been discussed by Stern[5] for silicon metal-oxide-semiconductor (MOS) inversion layers. Quantum wells were considered only very recently.[6]

Surprisingly, for one-dimensional systems such calculations have not yet been performed. The reason is probably that for Q1D ES analytical results for the electron-electron interaction potential are not available. In this paper we present results for the electron exchange and discuss the increase of the intersubband spacing due to direct Coulomb and exchange effects.

The total energy per electron, taking into account the kinetic energy ($\varepsilon_{\rm kin}$) and the exchange energy ($\varepsilon_{\rm ex}$) is also calculated. In the d-dimensional interacting electron gas one finds (for a review, see Ref. 7)

$$\varepsilon_{\rm ex}/\varepsilon_{\rm kin}=\begin{cases}-0.414r_s & \text{for } d=3\\ -1.200r_s & \text{for } d=2\ ,\end{cases} \tag{1}$$

where r_s is the density parameter. Exchange effects are more important in two dimensions than in three dimensions. Therefore, we expect that exchange effects are even more important in Q1D ES.

The paper is organized as follows. In Sec. II we describe the model. The result for the self-energy and the ground-state energy are presented and discussed in Sec. III. The summary is in Sec. IV.

II. MODEL

Analytical results for the subband spacings in Q1D ES (neglecting many-body effects) are only available for wires with rectangular or circular cross sections and for infinite barrier height. However, even for such simple models no analytical expressions are available for the electron-electron interaction potential $V^{ee}_{ijkl}(\mathbf{q})$. i, j, k, and l are subband indices.[4]

We have calculated the electron-electron interaction potential for a cylindrical quantum wire with radius R_0 and infinite barrier height at R_0. For this model the wave functions are expressed in terms of Bessel functions[8] and the energies of the two lowest subbands are given by

$$E_1=(5.78\ \text{Ry}^*)[a^*/R_0]^2$$

and

$$E_2=(14.68\ \text{Ry}^*)[a^*/R_0]^2\ .$$

$a^*=\varepsilon_L\hbar^2/me^2$ is the effective Bohr radius and $1\ \text{Ry}^*=me^4/2\varepsilon_L^2\hbar^2$ is the effective rydberg. m is the electron mass in the semiconductor and ε_L is the dielectric constant of the background. The intersubband energy $E^{(0)}_{21}=E_2-E_1$ is given by

$$E^{(0)}_{21}=(8.90\ \text{Ry}^*)[a^*/R_0]^2\ . \tag{2}$$

Using a simple approximation for the wave functions $\Phi(r,\phi)$ in the wire ($r\le R_0$) we are able to get analytical results for the electron-electron interaction potentials. For the wave function of the first subband we use $\Phi(r,\phi)\sim(1-r^2/R_0^2)$ and for the wave function of the second subband we use

$$\Phi(r,\phi)\sim r(1-r^2/R_0^2)e^{\pm i\phi}\ ,$$

see Ref. 9, and we get

$$V^{ee}_{1111}(\mathbf{q})=72\frac{e^2}{\varepsilon_L(qR_0)^2}\left[\frac{1}{10}-\frac{2}{3(qR_0)^2}+\frac{32}{3(qR_0)^4}-\frac{64}{(qR_0)^4}I_3(qR_0)K_3(qR_0)\right] \tag{3a}$$

and

$$V^{ee}_{1221}(\mathbf{q})=576\frac{e^2}{\varepsilon_L(qR_0)^2}\left[\frac{1}{60}-\frac{4}{15(qR_0^2)}+\frac{8}{(qR_0)^4}-\frac{64}{(qR_0)^4}I_4(qR_0)K_4(qR_0)\right]. \tag{3b}$$

$I_n(x)$ and $K_n(x)$ are modified Bessel functions.[10] For $qR_0 \ll 1$ we get

$$V^{ee}_{1111}(qR_0 \ll 1)=-2\frac{e^2}{\varepsilon_L}\ln\left[\frac{qR_0}{2}\right][1-O(q^2)] \tag{4a}$$

and

$$V^{ee}_{1221}(qR_0 \ll 1)=\frac{8e^2}{7\varepsilon_L}\left[1+\tfrac{3}{16}(qR_0)^2\ln\left[\frac{qR_0}{2}\right]+O(q^2)\right]. \tag{4b}$$

We have compared Eq. (3) with the exact (numerical) results (where we used the exact wave functions[8] for the calculation of the electron-electron interaction potentials) and we found very good agreement (within 5%).[9] In the following we use Eq. (3) for the electron-electron interaction potentials.

We consider a homogeneous electron gas (jellium model) with electron density $N=2g_v k_F/\pi=\hat{N}N_0$ and $N_0=1/2a^*$. g_v is the valley degeneracy, k_F is the Fermi wave number, and $\hat{N}$ is the reduced density. The density parameter r_s (Ref. 7) is given by $r_s=1/\hat{N}$ ($N=1/2r_s a^*$). A spin degeneracy of two is assumed. In the following we use $g_v=1$. All calculations are for zero temperature.

It is well known that shape effects of the wire cross section do not play an important role for the binding energies of hydrogenic impurities in one-dimensional systems.[11] We expect that the same is true for the exchange energies because the interaction potential is averaged over the wave functions.[4] In Ref. 12 $V^{ee}_{1221}(\mathbf{q})$ has been calculated for a quantum wire with zero thickness along one confined direction. The long-wavelength limit

$$V^{ee}_{1221}(\mathbf{q}=\mathbf{0})\approx 1.2e^2/\varepsilon_L$$

(Ref. 12) is in good agreement with our result, compare with Eq. (4b). Therefore, we believe that our model represents a generic model for the study of exchange effects in quasi-one-dimensional systems.

In our calculation we use the effective-mass approximation. Therefore, we expect that our theory is only valid for quantum wires which are not too thin: $2R_0 > a^*$. Because we used a confinement with infinite barriers we are restricted to widths of the quantum wire where

$$E_1=(5.8\ \text{Ry}^*)(a^*/R_0)^2 \ll V_0$$

and V_0 is the confinement energy in real wires. In semiconductor quantum wires with $1\text{Ry}^* \sim 5$–20 meV and V_0 of the order of 0.4–1.0 eV our restriction $2R_0 > a^*$ is safe enough to make our results applicable to real systems. The condition that only the lowest subband is occupied implies that the Fermi energy ε_F must be smaller than the intersubband energy distance E_2-E_1. From this condition it follows that $\hat{N} < 4a^*/R_0$.

III. RESULTS AND DISCUSSION

A. Self-energy

The exchange self-energy $\Sigma^{(1)}_{ex}(\mathbf{k})$ for the lowest subband is expressed in terms of $V^{ee}_{1111}(\mathbf{q})$ and given by

$$\Sigma^{(1)}_{ex}(\mathbf{k})=-\int_{-\infty}^{\infty}\frac{d\mathbf{q}}{2\pi}V^{ee}_{1111}(\mathbf{q})\Theta(k_F-|\mathbf{k}-\mathbf{q}|). \tag{5a}$$

$\Theta(x)$ is the unit-step function. The exchange energy $\Sigma^{(2)}_{ex}(\mathbf{k})$ for the second subband can be calculated following the derivation for two-dimensional systems.[13] In Ref. 13 $\Sigma^{(2)}_{ex}(\mathbf{k})$ was neglected. However, in Ref. 6 asymptotic results for $\Sigma^{(2)}_{ex}(\mathbf{k})$ have been presented for quantum wells. We get

$$\Sigma^{(2)}_{ex}(\mathbf{k})=-\int_{-\infty}^{\infty}\frac{d\mathbf{q}}{2\pi}V^{ee}_{1221}(\mathbf{q})\Theta(k_F-|\mathbf{k}-\mathbf{q}|). \tag{5b}$$

With Eq. (4) we derive for $k_F R_0 \ll 1$

$$\Sigma^{(1)}_{ex}(\mathbf{k})/(1\ \text{Ry}^*)=-\frac{N}{N_0}\left[1-\frac{k}{2k_F}\ln\left|\frac{k+k_F}{k-k_F}\right|-\tfrac{1}{2}\ln[|(k^2-k_F^2)|R_0^2/4]\right] \tag{6a}$$

and

$$\Sigma^{(2)}_{ex}(\mathbf{k})/(1\ \text{Ry}^*)=-\frac{4}{7}\frac{N}{N_0}\left\{1+\frac{(k_F R_0)^2}{32}\left[\left[1+\frac{k}{k_F}\right]^3\ln\left[\left|\frac{k+k_F}{2}\right|R_0\right]+\left[1-\frac{k}{k_F}\right]^3\ln\left[\left|\frac{k-k_F}{2}\right|R_0\right]-2\frac{k^2}{k_F^2}-\frac{2}{3}\right]\right\}. \tag{6b}$$

For $k_F R_0 \ll 1$ we get

$$\Sigma_{ex}^{(1)}(k_F)/(1\ \mathrm{Ry}^*) = -[N/N_0](1-\ln[k_F R_0]+\cdots) \quad (7a)$$

and

$$\Sigma_{ex}^{(2)}(k_F)/(1\ \mathrm{Ry}^*) = -\frac{4N}{7N_0}[1+\tfrac{1}{4}(k_F R_0)^2(\ln[k_F R_0]-\tfrac{1}{3})+\cdots]\ . \quad (7b)$$

$\Sigma_{ex}^{(1)}$ versus k given by Eq. (5a) is shown in Fig. 1, together with $\Sigma_{ex}^{(1)}$ given by Eq. (6a). As for three-dimensional systems (see, e.g., Ref. 14), we get with Eqs. (3a) and (5a) a divergent effective mass m^* at the Fermi points ($\pm k_F$):

$$m/m^* = 1+\frac{1}{\pi a^* k}\ln\left|\frac{k+k_F}{k-k_F}\right| . \quad (8)$$

We expect that, as for three-dimensional systems,[14] this singularity is canceled by correlation effects. But to the best of the authors' knowledge it has not previously been shown that the exchange contribution to the self-energy for Q1D ES gives a logarithmic singularity for the effective mass.

In Fig. 2 we show $\Sigma_{ex}^{(1)}(k_F)$ and $\Sigma_{ex}^{(2)}(k_F)$ versus electron density for various values of R_0. The dashed lines are for $k=0$. For small-electron density the self-energies increase with increasing electron density and become nearly constant for high-electron density. The self-energies depend strongly on the wire radius.

In Fig. 3 we show $\Sigma_{ex}^{(1)}(k_F)$ and $\Sigma_{ex}^{(2)}(k_F)$ versus wire radius R_0 for various values of N. The dashed lines are for $k=0$. The exchange self-energies decrease with increasing wire radius. However, the ratio $\Sigma_{ex}^{(1)}(k_F)/E_{21}^{(0)}$ increases with increasing wire radius. For $N/N_0=4$ we get for $\Sigma_{ex}^{(1)}(k_F)/E_{21}^{(0)}$ 0.10 (for $R_0=a^*/2$), 0.23 (for $R_0=a^*$), 0.49 (for $R_0=2a^*$), and 1.0 (for $R_0=4a^*$). We conclude that for large wire radii the exchange effects due to $\Sigma_{ex}^{(1)}(k_F)$ are of the same order as the intersubband

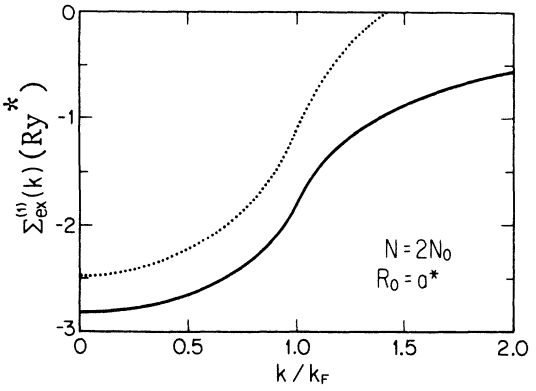

FIG. 1. Exchange self-energy $\Sigma_{ex}^{(1)}(k)$ vs wave number k (solid line). The dotted line represents Eq. (6a).

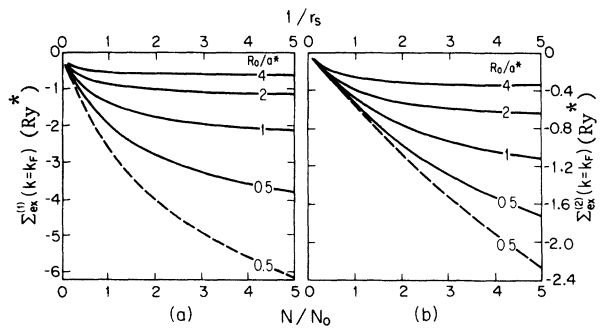

FIG. 2. (a) $\Sigma_{ex}^{(1)}(k=k_F)$ and (b) $\Sigma_{ex}^{(2)}(k=k_F)$ vs electron density N for various wire radii R_0. The dashed lines are for $k=0$, see Eq. (9).

energy-distance. $\Sigma_{ex}^{(2)}(k_F)$ is about a factor 5 smaller than $\Sigma_{ex}^{(1)}(k_F)$.

For different wire radii the exchange energies for $k=0$ and $k=k_F$ are related via

$$\Sigma_{ex}^{(i)}(k=0, 2R_0)=\Sigma_{ex}^{(i)}(k=k_F, R_0) \quad (9)$$

and $i=1,2$. With this relation one can get $\Sigma_{ex}^{(1)}(k=0)$ and $\Sigma_{ex}^{(2)}(k=0)$ from Figs. 2 and 3 (see the dashed lines).

Correlation contributions to the self-energies are not considered in this paper. From two-dimensional systems one knows[13] that the correlation contributions from the first subband and the second subband are comparable and the effect on the intersubband energy distance is small. The correlation contributions to the self-energies have a real and an imaginary part[15] making the interpretation in terms of a renormalization of the intersubband energy distance more complicated. The correlation contributions will be addressed elsewhere.[16]

B. Intersubband energy distance

The exchange self-energy gives rise to a renormalization of the intersubband energy distance $E_{21}^{(R)}(\mathbf{k})$ given by

$$E_{21}^{(R)}(\mathbf{k})=E_{21}^{(0)}-\delta E_{21}(\mathbf{k}) \quad (10a)$$

and

$$\delta E_{21}(\mathbf{k})=\Sigma_{ex}^{(1)}(\mathbf{k})-\Sigma_{ex}^{(2)}(\mathbf{k})+E_{21}^{BB}\ . \quad (10b)$$

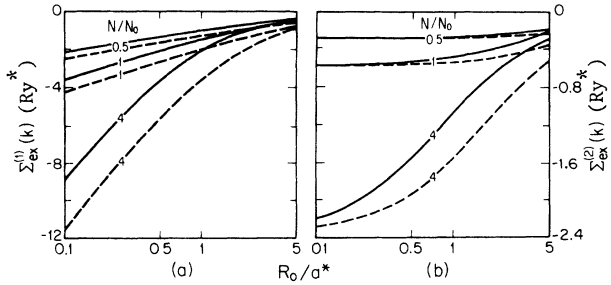

FIG. 3. (a) $\Sigma_{ex}^{(1)}(k=k_F)$ and (b) $\Sigma_{ex}^{(2)}(k=k_F)$ vs wire radius R_0 for various electron densities N. The dashed lines are for $k=0$, see Eq. (9).

We have assumed that the first subband is partially occupied and the second subband is unoccupied. E_{21}^{BB} is a renormalization of the intersubband energy distance due to band bending (BB). For small-electron concentration self-consistence effects in the Poisson equation are negligible. Thus, one can get analytical expressions for the change of the subband energies δE_i [$\delta E_1/(1\ \mathrm{Ry}^*)=1.22N/N_0$, $\delta E_2/(1\ \mathrm{Ry}^*)=0.90N/N_0$].[9] The change of the subband energy distance due to the Hartree-term is

$$E_{21}^{BB}/(1\ \mathrm{Ry}^*)=0.32N/N_0\ . \tag{10c}$$

E_{21}^{BB} does not depend on the wire radius. In Fig. 4 we show $\delta E_{21}(k=0)$ and $\delta E_{21}(k=k_F)$ versus electron density for $R_0=a^*$ according to Eq. (10). $|\delta E_{21}(\mathbf{k})|$ is strongly reduced for large N in comparison to $|\Sigma_{ex}^{(1)}|$ due to $\Sigma_{ex}^{(2)}$ and E_{21}^{BB}.

Presently, the experimentally studied wires[17–21] have large radii and exchange effects are certainly very important for the interpretation of intersubband energy distances. However, in most of the experiments three or more subbands are occupied making the interpretation of the experimental results difficult.

The intersubband energy distance ω_{21} measured by far-infrared optical spectroscopy[17,18,21] is shifted by the depolarization effect.[4] The long-wavelength limit is given by

$$\omega_{21}(\mathbf{k}=0)=\{[E_{21}^{(R)}(\mathbf{k}=0)]^2+[\Omega_{dp}(\mathbf{k}=0)]^2\}^{1/2}\ . \tag{11a}$$

The depolarization shift for quasi-one-dimensional systems has been calculated recently.[9,12] For our model we get

$$\frac{[\Omega_{dp}(\mathbf{k}=0)]^2}{[E_{21}^{(R)}(\mathbf{k}=0)]^2}=\frac{32}{7}\frac{Na^*}{[E_{21}^{(R)}(\mathbf{k}=0)/(1\ \mathrm{Ry}^*)]}\ . \tag{11b}$$

In Eq. (11) the renormalized energy distance $E_{21}^{(R)}$ enters and not $E_{21}^{(0)}$. For small-electron density $E_{21}^{(R)}>E_{21}^{(0)}$ and we conclude that the depolarization effects are larger if exchange and band bending are included in the calculation. In the former calculations[9,12] for the depolarization-shifted intersubband energy distance the exchange and band-bending effects have been neglected.

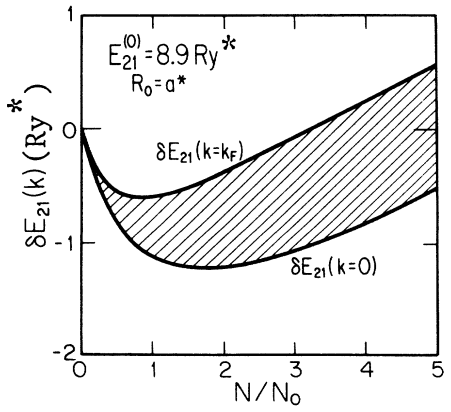

FIG. 4. $\delta E_{21}(k=0)$ and $\delta E_{21}(k=k_F)$ vs N for $R_0=a^*$, see Eq. (10b).

C. Ground-state energy

The ground-state energy per particle is written as[14]

$$\varepsilon=\varepsilon_{kin}+\varepsilon_{ex}+\varepsilon_{corr}\ . \tag{12}$$

ε_{corr} is due to correlation and is neglected in this paper. ε_{kin} is the kinetic energy per particle and given by

$$\varepsilon_{kin}=(1\ \mathrm{Ry}^*)\pi^2/(48r_s^2)=(0.2056...\ \mathrm{Ry}^*)/r_s^2\ . \tag{13a}$$

ε_{ex} is the exchange energy per particle and expressed as

$$\varepsilon_{ex}=\frac{1}{\pi N}\int_0^{k_F}d\mathbf{k}\,\Sigma_{ex}^{(1)}(\mathbf{k})\ . \tag{13b}$$

For $k_FR_0\ll 1$ ($r_sa^*/R_0\gg 1$) we get with Eq. (6a) the analytical expression

$$\varepsilon_{ex}/(1\ \mathrm{Ry}^*)=-[\ln(r_s)+\tfrac{3}{2}+\ln(4a^*/\pi R_0)]/[2r_s]\ . \tag{14}$$

In Fig. 5 we show ε_{kin}, ε_{ex}, and $\varepsilon_{kin}+\varepsilon_{ex}$ versus electron density N for $R_0=a^*/2$ and $R_0=a^*$. The inclusion of ε_{corr} and the comparison with ground-state energies of nonjellium ground states will certainly give new information on possible phase transitions. We mention that the occurrence of the Peierls transition was recently questioned for long-range Coulomb potentials.[22] It is clearly seen in Fig. 5 that the exchange energy is more important for Q1D ES than in higher dimensions: For $r_s=1$ we obtain $\varepsilon_{ex}/\varepsilon_{kin}=-6.1$ for $R_0=a^*/2$ and $\varepsilon_{ex}/\varepsilon_{kin}=-4.3$ for $R_0=a^*$. From Eq. (1) we get $\varepsilon_{ex}/\varepsilon_{kin}=-0.41$ for $d=3$ and -1.20 for $d=2$. For $r_sa^*/R_0\gg 1$ we find

$$\varepsilon_{ex}/\varepsilon_{kin}=-(2.432...)r_s[\ln(r_s)+\tfrac{3}{2}+\ln(4a^*/\pi R_0)]\ . \tag{15}$$

Comparing Eq. (15) with Eq. (1) we find that first the prefactor of the r_s^1 term is enhanced and that second an additional singular $\ln(r_sa^*/R_0)$ behavior is present for Q1D ES. Equation (15) demonstrates that exchange

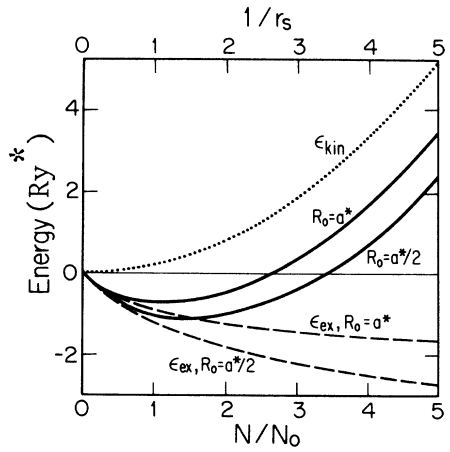

FIG. 5. ε_{kin} (dotted line), ε_{ex} (dashed lines), and $\varepsilon_{kin}+\varepsilon_{ex}$ (solid lines) vs electron density N for $R_0=a^*/2$ and $R_0=a^*$.

effects are strongly enhanced in Q1D ES in comparison to electron gases in higher dimensions.

IV. SUMMARY

To summarize, the exchange energy for quasi-one-dimensional wires was calculated and the renormalization of the intersubband energy distance due to Coulomb and exchange interactions was evaluated. The implications of our calculations for future experiments on quasi-one-dimensional wires, where only one subband is partially filled, are evident and important.

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