Exchange energy for electrons in two dimensions: Effects of finite temperature and finite thickness

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(Received 5 December 1994)

The effects of finite temperature and finite thickness on the exchange energy for a two-dimensional system of electrons such as those confined in quantum wells are evaluated and expressed as a parametrized correction factor $[1 + (\pi^2/16)\tau^2 \ln \tau - 0.874\tau^2 + 1.786\tau^3] - 0.109\kappa + 0.0076\kappa^2$ for $0 < \tau < 0.4$ and $0 < \kappa < 5.5$. Here $\tau = k_B T/(\hbar^2 K_F^2/2m^*)$ is the ratio of thermal energy to the Fermi energy and $\kappa = K_F L$, K_F and L being the two-dimensional Fermi wave number and the thickness, respectively. The absolute value of the (negative) exchange energy is decreased by these effects.

Recent progress in semiconductor technologies has provided us with a variety of nanostructures as fields for research in fundamental physics and as useful elements for electronic devices. One of the simplest and the most important structures may be the one-dimensional quantum well which enables us to realize two-dimensional systems of electrons. There have been proposed many devices with new functions based on this structure where the effects coming from the many-body interactions between electrons sometimes play an important role. A typical example may be the modification of energy levels due to accumulation of carriers:[1] Among various elements affecting the level structure,[2] the mean-field (Hartree) and the exchange-correlation interaction are responsible for this modification.

In many cases the Kohn-Sham formulation of the density-functional theory[3] has been applied. In these analyses of electronic states, many-body interactions are described by the mean-field (Hartree) and the exchange-correlation potentials. In the Kohn-Sham equation, the Hartree potential is given exactly by solving the Poisson equation for the charge distribution. The geometrical effect can be taken into account by employing appropriate numerical procedures such as the finite element method, if necessary. The exchange-correlation potential, however, has to be determined through some approximate expression in terms of the density. The purpose of this paper is to give possible modifications in a parametrized form useful for such formulations.

When we neglect both the temperature and thickness of the well and regard our system of electrons as purely two dimensional, we may apply the results of numerical experiments on two-dimensional electron liquids at $T = 0$ of Tanatar and Ceperley.[4] For two-dimensional electrons in GaAs, however, the Fermi temperature at the typical density of 10^{11}cm^{-2} is about 40 K and the effect of finite temperature may not be negligible even at 4.2 K.

When we denote the planar density of electrons by N_s, the application of two-dimensional results may be valid if the two-dimensional mean distance $(\pi N_s)^{-1/2}$ of electrons is sufficiently larger than the thickness of the well L or, in terms of the two-dimensional Fermi wave number $K_F = (2\pi N_s)^{1/2}$,

$$\kappa = K_F L \ll 1. \tag{1}$$

The characteristic distance of the correlation between electrons in the plane is $(\pi N_s)^{-1/2}$ and (1) means that L can be neglected at this distance. In many cases, however, the value of the left-hand side does not seem to be negligibly small; $N_s \sim 10^{11}$ cm^{-2} and $L \sim 5 \times 10$ Å gives $\kappa = 0.4$. In this paper, we will give the exchange energy between electrons in quantum wells for finite temperatures and finite thicknesses in a parametrized form.

The (first-order) exchange energy is given by[5]

$$U_{\text{ex}} = -\frac{1}{2\varepsilon} \sum_{\alpha_1} \sum_{\alpha_2} \sum_{\sigma} n_{\alpha_1 \sigma} n_{\alpha_2 \sigma} \int\int d\mathbf{r}_1 d\mathbf{r}_2 \psi_{\alpha_2}^*(\mathbf{r}_1)$$
$$\times \psi_{\alpha_1}^*(\mathbf{r}_2) \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \psi_{\alpha_1}(\mathbf{r}_1) \psi_{\alpha_2}(\mathbf{r}_2). \tag{2}$$

Here the spatial part of the one-particle state $\psi(\mathbf{r})$ is indexed by α and $n_{\alpha\sigma}$ is the occupation number of the state (α, σ), σ being the spin, and ε is the dielectric constant.

When electrons are in a quantum well perpendicular to z and we denote the coordinates parallel to the well by $\mathbf{R}$ as $\mathbf{r} = (\mathbf{R}, z)$, electronic states (envelope functions) are given by

$$\psi_{\mathbf{K},i}(\mathbf{R}, z) = \frac{1}{S^{1/2}} \exp(i\mathbf{K} \cdot \mathbf{R})\phi_i(z). \tag{3}$$

Here the area S is the system size along the well and indices of these states are the two-dimensional wave number $\mathbf{K}$ and the index i of (normalized) eigenstates with respect to z. In what follows, we assume that electrons are in the ground state $\phi_0(z)$ with respect to the motion in the z direction. Substitution of this wave function into (2) gives

$$U_{\text{ex}} = -\frac{1}{2\varepsilon} \sum_{\mathbf{K}_1} \sum_{\mathbf{K}_2} \sum_{\sigma} n_{\mathbf{K}_1\sigma} n_{\mathbf{K}_2\sigma} \frac{1}{S^2} \int\int d\mathbf{R}_1 d\mathbf{R}_2 \exp[i\mathbf{K}_{12} \cdot (\mathbf{R}_1 - \mathbf{R}_2)] \int\int dz_1 dz_2 |\phi_0(z_1)|^2 |\phi_0(z_2)|^2 \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \quad (4)$$

with $\mathbf{K}_{12} = \mathbf{K}_1 - \mathbf{K}_2$. Since $(\mathbf{r}_1 - \mathbf{r}_2)^2 = (\mathbf{R}_1 - \mathbf{R}_2)^2 + (z_1 - z_2)^2$, the above expression reduces to

$$U_{\text{ex}} = -\frac{e^2}{2\varepsilon S} \sum_{\mathbf{K}_1} \sum_{\mathbf{K}_2} \sum_{\sigma} n_{\mathbf{K}_1\sigma} n_{\mathbf{K}_2\sigma} \int\int dz_1 dz_2 \frac{2\pi}{K_{12}} \exp(-K_{12}|z_1 - z_2|) |\phi_0(z_1)|^2 |\phi_0(z_2)|^2. \quad (5)$$

For $\phi_0(z)$ we use an approximation

$$\phi_0(z) = (2/L)^{1/2} \cos(\pi z/L), \qquad -L/2 < z < L/2. \quad (6)$$

This approximation may be justified a posteriori by the fact that our result gives a correction typically of the order of 10%. After integrating with respect to z_1 and z_2, we have

$$U_{\text{ex}} = -\frac{e^2}{2\varepsilon S} \sum_{\mathbf{K}_1} \sum_{\mathbf{K}_2} \sum_{\sigma} n_{\mathbf{K}_1\sigma} n_{\mathbf{K}_2\sigma} \frac{2\pi}{K_{12}} \left\{ \frac{2}{1 + (K_{12}L/2\pi)^2} \left[\frac{1}{K_{12}L} + \frac{3}{8\pi^2} K_{12}L - \frac{1}{(K_{12}L)^2} \frac{1 - \exp(-K_{12}L)}{1 + (K_{12}L/2\pi)^2} \right] \right\}. \quad (7)$$

When $L = 0$, the expression in curly brackets reduces to unity.

At $T = 0$, $n_{\mathbf{K}\sigma} = \theta(K_F - K)$ and the exchange energy has been given as[6]

$$U_{\text{ex}}(L = 0, T = 0)/SN_s = -(4\sqrt{2}/3\pi)(\pi N_s)^{1/2}. \quad (8)$$

The effect of finite thickness is expressed by the ratio $U_{\text{ex}}(L, T = 0)/U_{\text{ex}}(L = 0, T = 0)$ which is a function of κ. Values of this ratio are shown in Fig. 1 and can be interpolated by a formula

$$\frac{U_{\text{ex}}(L, T = 0)}{U_{\text{ex}}(L = 0, T = 0)} = 1 - 0.109\kappa + 0.0076\kappa^2$$

$$\text{for} \quad 0 < \kappa < 5.5 \quad (9)$$

with relative errors less than 1%.

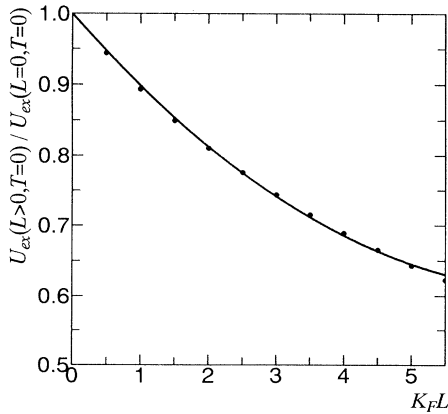In the case of $L = 0$, it is easily seen that the leading term of the finite-temperature effect is proportional to $T^2 \ln T$. The coefficient is calculated as

$$\frac{U_{\text{ex}}(L = 0, T > 0)}{U_{\text{ex}}(L = 0, T = 0)} = 1 + \frac{\pi^2}{16} \tau^2 \ln \tau + O(\tau^2), \quad (10)$$

where $\tau = k_B T/(\hbar^2 K_F^2/2m)$. We numerically evaluate the values of $U_{\text{ex}}(L = 0, T)/U_{\text{ex}}(L = 0, T = 0)$ for small values of τ and express the results by an interpolation formula

$$\frac{U_{\text{ex}}(L = 0, T > 0)}{U_{\text{ex}}(L = 0, T = 0)} = 1 + \frac{\pi^2}{16} \tau^2 \ln \tau - 0.874\tau^2 + 1.786\tau^3$$

$$\text{for} \quad 0 < \tau < 0.4 \quad (11)$$

as shown in Fig. 2. The relative error of this expression is less than 1%. The exchange energy is decreased by the finite-temperature effect. It should be noted that the term proportional to τ^3 is adopted only for numerical

FIG. 1. Effect of finite thickness. Absolute value of the first-order exchange energy is reduced by this factor depending on $K_F L$, K_F and L being the two-dimensional Fermi wave number and width of the well, respectively.
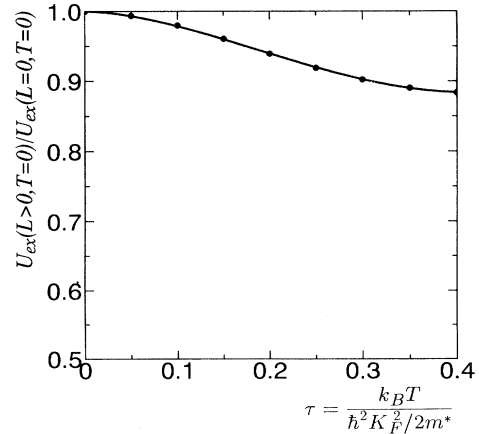

FIG. 2. Effect of finite temperature. Absolute value of the first-order exchange energy is reduced by this factor depending on $k_B T/(\hbar^2 K_F^2/2m^*)$, T and $\hbar^2 K_F^2/2m^*$ being the temperature and the Fermi energy, respectively.
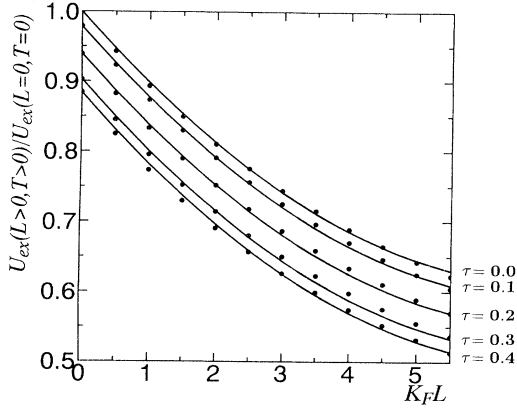
FIG. 3. Reduction factor for finite temperature and finite thickness. Solid lines are interpolations for numerical results shown by dots with $k_B T/(\hbar^2 K_F^2/2m^*) = 0$, 0.1, 0.2, 0.3, and 0.4.
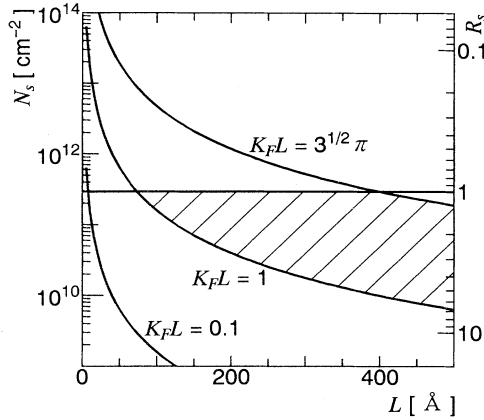

FIG. 4. Applicability of our result. In the hatched area, the exchange effect is important and our correction factor is substantial.
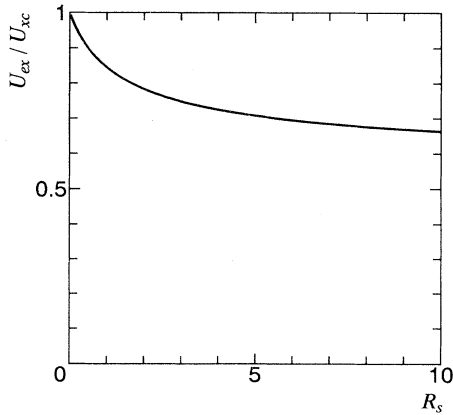

FIG. 5. Contribution of first-order exchange energy $U_{\rm ex}$ in total exchange-correlation energy $U_{\rm xc}$ at $T = 0$. It is still dominant for R_s as large as 10.

purposes and the expansion with respect to τ may include such terms as $\tau^3 \ln^2 \tau$.

Both finiteness of temperature and finiteness of thickness reduce the absolute value of the exchange energy. We also evaluate the ratio $U_{\rm ex}(L,T)/U_{\rm ex}(L = 0, T = 0)$ in the case where they are finite at the same time. The results are shown in Fig. 3 and approximately interpolated by simply shifting the value for $\kappa = 0$ as

$$\frac{U_{\rm ex}(L > 0, T > 0)}{U_{\rm ex}(L = 0, T = 0)} = \left[1 + \frac{\pi^2}{16}\tau^2 \ln \tau - 0.874\tau^2 + 1.786\tau^3\right]$$
$$-0.109\kappa + 0.0076\kappa^2$$

$$\text{for } 0 < \tau < 0.4 \text{ and } 0 < \kappa < 5.5 \quad (12)$$

with relative errors less than 2%.

Let us now discuss the applicability of our result. We have assumed that only the ground state with respect to z is occupied by our electrons. This gives an upper limit for the electron density

$$\hbar^2 K_F^2/2m^* \leq (2^2 - 1)(\hbar^2/2m^*)\left(\frac{\pi}{L}\right)^2 \quad (13)$$

or

$$\kappa \leq 3^{1/2}\pi, \quad (14)$$

which is plotted in Fig. 4. In order for the exchange effect to play an important role, the parameter $R_s = 1/(\pi N_s)^{1/2}a_B$ of two-dimensional electrons needs to be larger than unity ($a_B = \varepsilon\hbar^2/m^*e^2$ is the Bohr radius). We plot the condition $R_s = 1$ in Fig. 4 for electrons in GaAs ($m^*/m_e = 0.067$ and $\varepsilon = 13$). In Fig. 4 we also plot the conditions $\kappa = 1$ and $\kappa = 0.1$. We see that our correction factor is applicable and also significant in the domain with shading which includes typical values of electron density and well thickness in experiments.

The above results are related to the first-order exchange energy. In Fig. 5 we plot the ratio of the first order exchange energy at $T = 0$ to the total exchange-correlation energy $U_{\rm xc}$ obtained by Tanatar and Ceperley.[4] Comparing Figs. 4 and 5, we may conclude that the first-order exchange energy is still the main part in the domain where our result applies.

Though exact values of the correlation energy at finite-temperatures are not known even for $L = 0$, the finite temperature effect is expected to be in the opposite direction to that on the exchange energy.[7,8] The finiteness of thickness, on the other hand, reduces the absolute values of both energies through modification of the Coulomb potential. In our parameter domain, the latter may be the main effect as shown in Fig. 3 and the former will be weakened further due to partial cancellation when the correlation energy is taken into account.

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