Ground State of Coupled Quantum Wires

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SYNOPSIS

The ground states of interacting electrons in coupled quantum wires are analyzed on the basis of the density functional theory. The exchange-correlation potential is calculated from 'exact' results given by the Green's function Monte Carlo method in two and three dimensions. It is shown that the critical density signifying the change from symmetrical to asymmetrical ground state is weakly dependent on the details of the exchange-correlation potential. These critical values are compared with the result of the three-dimensional analysis for a single wire.

I. INTRODUCTION

When electronic levels in quantum wires or wells are occupied by many electrons, the interaction between electrons plays an important role in determining energy eigenvalues and distribution of electrons among them. The many body interaction between electrons may be accounted for by the repulsive electrostatic (Hartree) interaction and the attractive exchange-correlation interaction.

In symmetric or nearly symmetric structures composed of two quantum wires or wells, the symmetric distribution of electrons has the lowest electrostatic energy if

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the interactions between electrons are neglected. The Hartree energy per electron is proportional to the density of electrons. Additional electric fields between two wires or wells accompany asymmetric distributions and the total energy is increased by positive contributions from these additional Hartree fields which are also roughly proportional to the spacing between wires or wells. Symmetric distributions are thus further stabilized when we take the Hartree interaction into account.

The exchange-correlation interaction is attractive and its value per electron is proportional to the inverse of the mean distance between electrons. This part of the total energy generally decreases when the distribution becomes asymmetric due to nonlinear dependence on the density. When two quantum wells or wires are placed closely enough and the increase of the Hartree energy due to asymmetry is small, it may be possible that the decrease of the exchange-correlation energy overcomes the increase of the electrostatic energy. We then have electrons populating in either of the wires or wells, even if the structure is almost symmetric.

This kind of possibility has been first pointed out by Ruden and Wu[1, 2]. They have analyzed the stability of symmetrical distribution of electrons in two parallel two- or one-dimensional electron systems taking the Hartree energy and the first order exchange energy into account. In their analyses, two systems are regarded as independent except for interaction through the Hartree field and interference of wave functions or tunneling between two domains has been ignored.

The usefulness of this kind of phenomena may partly depend on how fast the electronic distribution can be reversed. From this point of view, the coupling between two wells or wires needs to be strong enough. Obviously, however, strong coupling may have an effect which favors symmetric ground state. We thus have to make some compromise between these two effects in opposite directions based on computations which seriously take into account the interference of wave functions in each domain. Calculations with full account of the coupling of wave functions have been done by the present authors[3].

In previous results, the mean distance between electrons is larger than the distance between two wells or wires when localized states become stable. We therefore cannot *a priori* rule out the possibility of the appearance of structures in the electronic distribution in the direction(s) along wires or parallel to layers and three-dimensional analyses are necessary at least in principle.

In this paper, we propose a structure composed of two quantum wells (or ribbon-like wires) laterally coupled through a narrow constriction with the cross section shown in Fig.1 and show that we have asymmetric ground state localized in either of wells under appropriate conditions. The localized distribution may be easily reversed by applying the electrostatic bias in the direction connecting two wells. We assume that our coupled wells containing electrons are surrounded first by neutral layers and then highly doped domains with high electron densities, and the overall charge neutrality is maintained by positive charges appearing on inner surfaces of the high density domains. These structures may be realized, for example, by modifying the concentration x of Al in $Al_xGa_{1-x}As$ and the doping profile of donors. The concentration profile, $x = 0$ in the well and $0 < x < 0.45$ otherwise, provides a potential barrier V_0 around the wells by the conduction band offset and the doping of donors only in outer domains will leave non-doped neutral layers around wells.
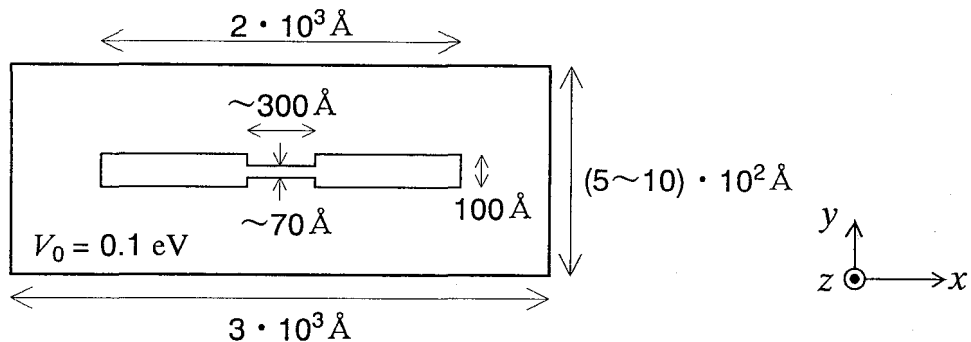

Fig.1. Cross section of coupled quantum wires.

II. FORMULATION

We apply the effective mass approximation with the effective mass $m^* = 0.067m_e$ (m_e being the electronic mass) for electrons in our system. The main purpose of this paper is to analyze the many-body effects of electrons and we expect those effects beyond the approximation may have small influence on main conclusions. We first assume that the distribution in the direction along wires is uniform and perform computations in two dimensions. We then ascertain the validity of this assumption by three-dimensional computations for a single well.

In order to describe many-body effects, we adopt the density functional theory in the local density approximation which is now one of standard procedures in these analyses. The exchange-correlation part of the interaction potential can be obtained from the results of numerical experiments. These 'exact' results based on the Green's function Monte Carlo method are now available for ground states of electrons in three and two dimensions due to Ceperley and Alder[4] and Tanatar and Ceperley[5], respectively. Three-dimensional values have been parametrized by Vosko et al.[6] The exchange-correlation potential $V_{xc}(\mathbf{r})$ is calculated by

$$V_{xc}(\mathbf{r}) = \frac{\delta E_{xc}[n(\mathbf{r})]}{\delta n(\mathbf{r})}, \tag{2.1}$$

where $E_{xc}[n(\mathbf{r})]$ is given, in the local density approximation, by

$$E_{xc}[n(\mathbf{r})] = \int d\mathbf{r}\, n(\mathbf{r}) \varepsilon_{xc}(n(\mathbf{r})) \tag{2.2}$$

with the exchange-correlation energy per electron in homogeneous system ε_{xc}.[6, 5] We denote these potentials by $V_{xc}^{(2d)}$ and $V_{xc}^{(3d)}$.

Following Kohn and Sham[7], the electronic levels $\{E_i\}$ are determined by

$$\left(-\frac{\hbar^2}{2m^*}\Delta + V_{ext}(\mathbf{r}) + V_C(\mathbf{r}) + V_{xc}(\mathbf{r}) \right) \psi_i(\mathbf{r}) = E_i \psi_i(\mathbf{r}), \tag{2.3}$$

and the density of electrons $n(\mathbf{r})$ is calculated by filling electrons into these eigenstates up to the Fermi level as

$$n(\mathbf{r}) = \sum_i |\psi_i(\mathbf{r})|^2. \tag{2.4}$$

The potential $V_{ext}(\mathbf{r})$ denotes the conduction band offset between the well and the surrounding neutral layer: $V_{ext} = 0$ in the well and $V_{ext} = V_0$ otherwise. In solving (2.3) the boundary condition $\psi_i(\mathbf{r}) = 0$ is imposed at inner surfaces of the high density domain. Actually, wave functions of bound states in wells completely decay before we apply this condition.

The electrostatic potential $V_C(\mathbf{r})$ is given by

$$V_C(\mathbf{r}) = e^2 \int \frac{n(\mathbf{r}') - n^+(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}', \qquad (2.5)$$

where $n^+(\mathbf{r})$ is the density of positive charges which neutralizes negative electronic charges in our wells. In our analysis we calculate $V_C(\mathbf{r})$ with $n^+(\mathbf{r}) = 0$ adopting the boundary condition $V_C(\mathbf{r}) = 0$ at the inner surfaces of the high density domain treating the latter as conductive (metallic).

Starting from some trial wave functions, we solve above equations self-consistently. As a numerical method, we apply the finite element method to compute the solution of the Schrödinger equation (2.3) and the Poisson equation (2.5) and self-consistency is attained by iteration.

III. ANALYSES IN TWO DIMENSIONS WITH V_{XC}^{2D} AND V_{XC}^{3D}

We have analyzed electronic states in our system in the cases of both two- and three-dimensional exchange-correlation potentials. The results are summarized in Figs.2~ 5.

For the two-dimensional case, the total energy per electron is plotted as a function of linear density of electrons in Fig.2. The values for symmetric ground state and the asymmetric ground states are equal at the critical density. For higher densities the symmetric ground state has lower energy and the asymmetric ground state is a local minimum in configuration space. For lower densities, the asymmetric ground state has lower energy and the symmetric ground state is a local minimum. The ground state thus changes from the symmetric state for high densities to asymmetric state for lower densities as shown in Fig.3.

The contribution of the Hartree part and the exchange-correlation part are shown in Fig.4a and 4b. We see that the former is proportional to the density and the latter, to $n^{1/2}$. The behavior of the Hartree part is in accordance with our expectation. The dependence of the exchange correlation energy on the density reflects that we have adopted the two-dimensional values.

Three-dimensional results are shown in Figs.5 and 6. We observe similar dependencies of energies on the density except for the exchange-correlation part which is proportional to $n^{1/3}$ in this case.
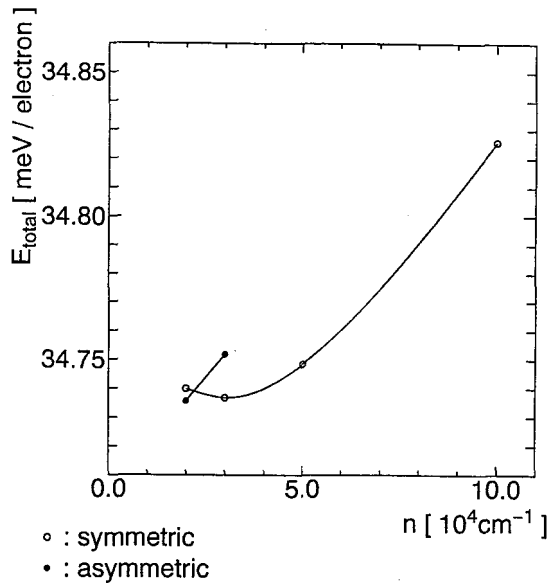
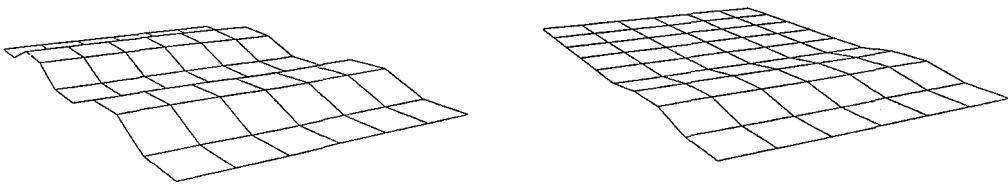Fig.2. Total energy per electron vs. density.

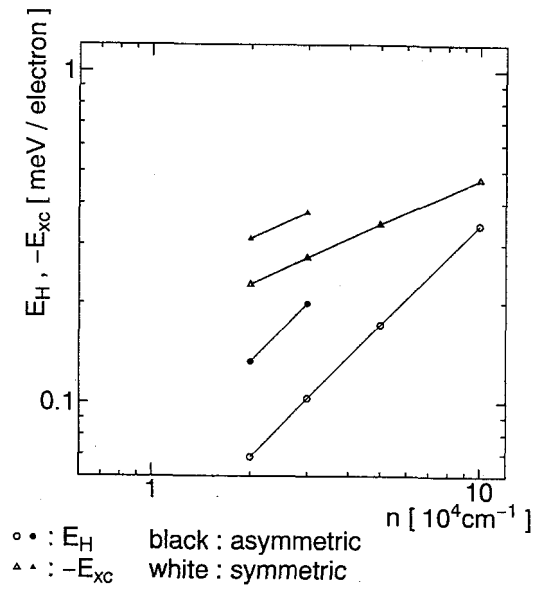Fig.3. Distribution of electrons in symmetric and asymmetric ground states. Both are uniform in z.

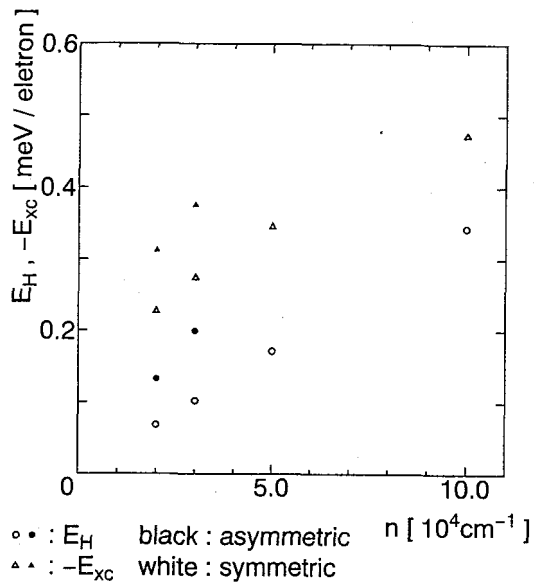**Fig.4a.** Hartree and exchange-correlation part of electronic energy vs. density.

Fig.4b. The same as Fig.4a in linear scale. Compare absolute values of differences in Hartree and exchange-correlation energy for symmetric and asymmetric states.
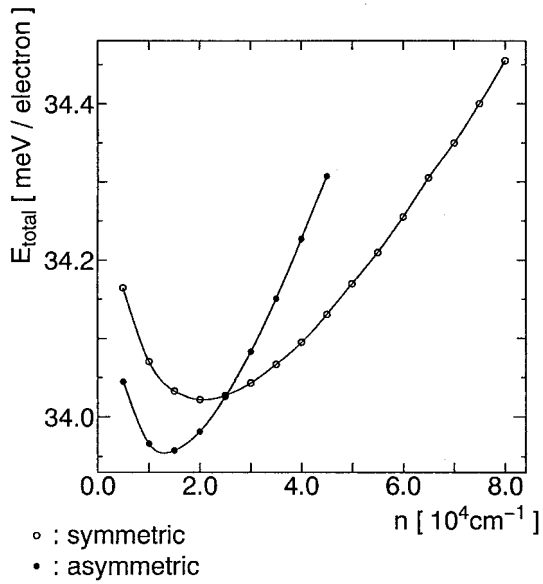
∘ : symmetric
• : asymmetric

Fig.5. Total energy per electron vs. density.

∘ • : E_H black : asymmetric
▲ ▲ : $-E_{xc}$ white : symmetric

∘ • : E_H black : asymmetric
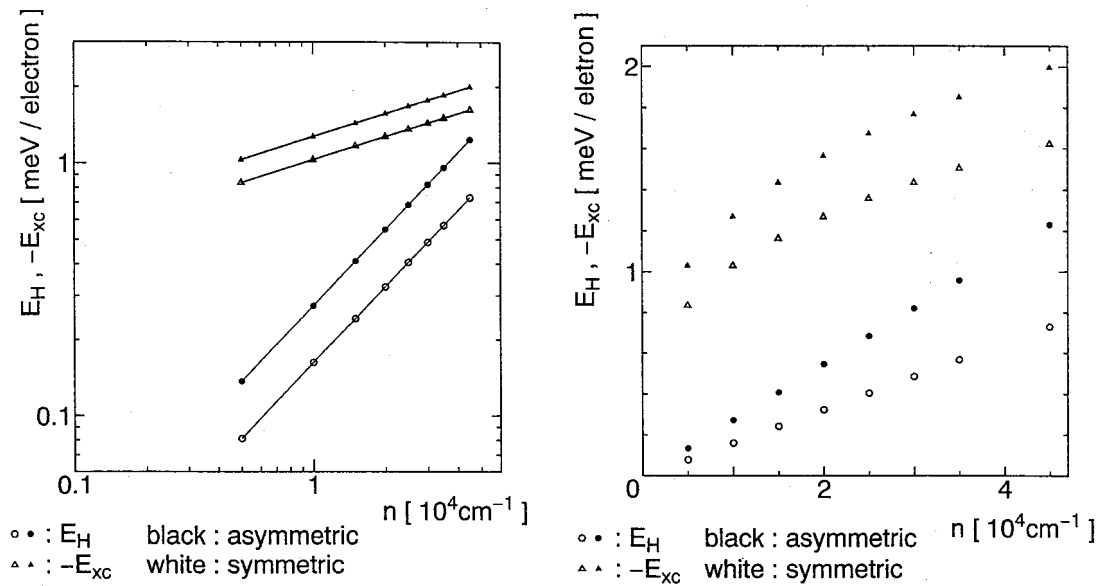▲ ▲ : $-E_{xc}$ white : symmetric

Fig.6a and 6b. Hartree and exchange-correlation part of electronic energy vs.

density.

The critical densities in the case of three- and two- dimensional exchange-correlation potentials are $2.5 \cdot 10^4 \mathrm{cm}^{-1}$ and $2.1 \cdot 10^4 \mathrm{cm}^{-1}$, respectively. We note that these results are very close. We therefore expect that details of the exchange-correlation energy do not have serious effect on the critical density. It should be also noted that the mean distance between electrons at the critical density is much larger than the thickness of our wells, 100Å. The application of two-dimensional result thus turns out to be more appropriate.

The mean distance between electrons is also much larger than the width of our ribbons, $2 \cdot 10^3$Å. To apply the two-dimensional results of the exchange-correlation potential therefore is not justified in the strict sense. We have, however, no 'exact' results for one-dimensional case and the results with two- and three-dimensional potentials are almost the same. We may thus adopt the two-dimensional values for the potential to obtain semi-quantitative results.

IV. ANALYSES IN THREE DIMENSIONS WITH V_{XC}^{2D} AND V_{XC}^{3D}

In order to ascertain the correctness of our assumption that the electronic density in the z-direction is uniform, we solve the Kohn-Sham equation in three dimensions. We confine electrons in a ribbon of length L_z in z-direction and impose the periodic boundary condition along the z-axis. The cross section of the ribbon is shown in Fig.7. We may expect that whether z-dependent structures in the electronic density appear or not does not depend on details of the geometry of the cross section of the wire.
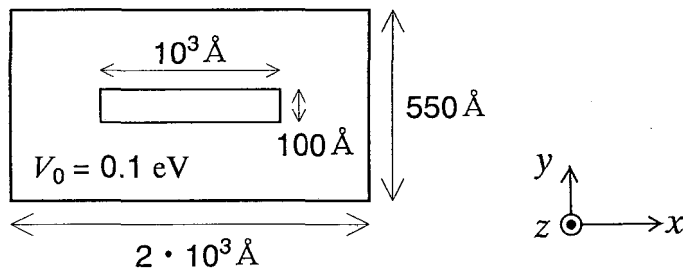

Fig.7. Cross section of quantum wire for three-dimensional analysis.

Value of parameters in three-dimensional analysis are summarized in Table 1. The distribution with structure in z is shown in Fig.8. We see that, in the domain of the linear density where the transition between symmetrical and asymmetrical ground states occurs, the uniform electronic density is obtained in three dimensional computations. We may therefore confirm the validity of two-dimensional analyses.

We have also performed similar analysis with three-dimensional exchange-correlation potential. The critical density obtained by the analysis in two dimensions is also larger than that obtained in three dimensions.

Table 1. Parameters in Three-Dimensional Analysis

number of electrons	length (L_z)[Å]	linear density $(2/L_z)$[cm^{-1}]	uniform/structure
2	10^4	$2 \cdot 10^4$	uniform
2	$1.5 \cdot 10^4$	$1.3 \cdot 10^4$	uniform
2	$2 \cdot 10^4$	$1 \cdot 10^4$	structure

V. CONCLUDING REMARKS

In these analyses, we have confined ourselves within the ground state. The Fermi energy of electrons with respect to the degree of freedom in z-direction may be estimated by

$$E_F = \frac{\pi^2 \hbar^2 n^2}{2m^*}, \tag{5.1}$$

which is 0.022meV or 0.26K at the critical density. Thus the temperature needs to be in this domain. The difference in energies per electron in symmetrical and asymmetrical states easily exceeds this value when the density is off the critical value by 10% as is shown in Fig.2.

This kind of phenomena may be regarded as the appearance of the Wigner lattice in restricted geometries. The value of the parameter r_s (in two dimensions) at the

critical density is around 16. This is smaller than the critical value for Wigner crystallization in two dimensions 37 ± 5 predicted by the numerical experiments[5] the results of which we have adopted as exchange-correlation potential. The difference may be due to the effect of geometry of our system.

Based on these results, we may expect the behavior of the electronic distribution in coupled quantum wires as follows: With the decrease of the linear density n, we have, symmetric distribution uniform in z when $n > n_{c2}$, asymmetric distribution uniform in z when $n_{c2} > n > n_{c3}$, and, asymmetric distribution structured in z when $n_{c3} > n$.

In conclusion, we have shown that electrons in the ground sate of coupled symmetrical quantum wires can be localized in either of wires when the linear density is lower than some critical value. Mainly responsible for this phenomenon is the exchange interaction between electrons which overcomes the increase of the Hartree energy due to localization at sufficiently low densities. Though the temperature needs to be low enough, this is the first result for realistic systems which confirms the previous expectation of this kind of phenomena in idealized cases.
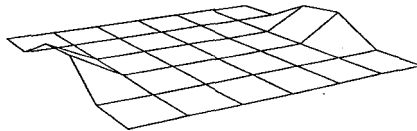

Fig.8. Ground state of electrons in quantum wire with structure in z direction.

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