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Intrinsic Bistability of Coupled Quantum Wires: Localization due to Many-Body Effects

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SYNOPSIS

The ground state of a system of electrons accumulated in a pair of coupled symmetric quantum wires is analyzed on the basis of density functional theory. It is shown that, in a domain of physical parameters, electrons are localized in either of wires. The main contribution to the total energy of this system comes from the Hartree energy, or the electrostatic energy, and the exchange-correlation energy between electrons. The ground state is determined by a competition between these contributions: We have symmetric electron distributions when the Hartree energy dominates and asymmetric (localized) states are realized in the opposite case. This kind of simple system with bistable electronic states may be applied to semiconductor memory devices.

I. INTRODUCTION

Owing to the development of technologies to control the crystal growth, there have been numerous proposals of semiconductor microstructures whose new or higher functions have now realistic meaning. In this paper, we show an interesting property

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of coupled quantum wires which may be utilized in electronic devices.

The essential part of the structure of our system is the quantum wires coupled through a thin tunneling barrier. The result of our calculation shows that, under appropriate conditions, electrons doped in this system localize in either of two wells. For simplicity and also considering applications, we may assume that two wells are symmetric. We also assume that the ionized donors are distributed symmetrically around the wells.

At first sight, it seems natural that electrons are symmetrically distributed since the Coulomb repulsion will keep them apart: In other words, the Hartree energy increases when electrons are asymmetrically distributed. On the other hand, the exchange and correlation energy of electrons is negative and its absolute value increases with the increase of the density with the power of one third (per electron). It is thus possible that the exchange-correlation energy as a whole decreases for asymmetric distributions and overcomes the increase of the Hartree energy.

It is expected that the distance between two wells needs to be very small; when regarded as a capacitor, the electrostatic energy of our system increases roughly in proportion to the mutual distance. We thus have to take the interference and tunneling between two wells into account seriously.

This kind of possibility has been first pointed out by Ruden and Wu[1, 2]. They analyzed the stability of symmetrical distribution in two parallel two- or one-dimensional electron systems with the first order exchange energy. In their analysis, however, two systems are assumed to be independent except for electrostatic interaction and the interference and tunneling between two electron systems have been completely neglected. In addition, the resultant mean distance between electrons in each system is larger than the distance between two systems. The treatment as independent electron systems therefore seems to fail at least quantitatively.

The purpose of this paper is to analyze the aforementioned possibility for realistic structures with full account for interference and tunneling based on more accurate

values of the exchange and correlation energy.

II. METHOD OF ANALYSIS AND FUNDAMENTAL EQUATIONS

We apply the effective mass approximation for electrons in our structure. 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.

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. As the functional describing the exchange and correlation energy, we use the parametrized form of Vosko *et al.*[3] based on the results of Ceperley and Alder[4] by the Green's function Monte Carlo method. Application of this zero temperature expression is justified *aposteriori* by the domain of density where the expected phenomenon occurs.

Following the method of Kohn and Sham[5], the electronic levels $\{E_i\}$ are determined by

$$\left(-\frac{\hbar^2}{2m^*}\Delta + V_0(\mathbf{r}) + V_C(\mathbf{r}) + V_{xc}(\mathbf{r})\right)\psi_i(\mathbf{r}) = E_i\psi_i(\mathbf{r}), \tag{2.1}$$

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

$$n(\mathbf{r}) = \sum_i |\psi_i(\mathbf{r})|^2. \tag{2.2}$$

The potential $V_0(\mathbf{r})$ denotes the conduction band offset between the well and the barrier or the surrounding wall. The electrostatic potential $V_C(\mathbf{r})$ is given by

$$V_C(\mathbf{r}) = e^2 \int \frac{n(\mathbf{r}') - n_D(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}', \tag{2.3}$$

where $n_D(\mathbf{r})$ is the density of ionized donors. The exchange-correlation potential $V_{xc}(\mathbf{r})$ is calculated by

$$V_{xc}(\mathbf{r}) = \frac{\delta E_{xc}[n(\mathbf{r})]}{\delta n(\mathbf{r})}, \tag{2.4}$$

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

$$E_{xc}[n(\mathbf{r})] = \int d\mathbf{r} n(\mathbf{r}) \varepsilon_{xc}(n\mathbf{r}), \tag{2.5}$$

with the exchange-correlation energy per electron in homogeneous system ε_{xc}. The latter energy at $T = 0$ is expressed as

$$\varepsilon_{xc}(r_s) = -\left(\frac{9\pi}{4}\right)^{1/3} \frac{3}{2\pi r_s} + A\left\{\ln\frac{x^2}{X(x)} + \frac{2b}{Q}\tan^{-1}\frac{Q}{2x+b} - \frac{bx_0}{X(x_0)}\left[\ln\frac{(x-x_0)^2}{X(x)} + \frac{2(b+2x_0)}{Q}\tan^{-1}\frac{Q}{2x+b}\right]\right\}, \tag{2.6}$$

$$x = r_s^{1/2}, \tag{2.7}$$

$$X(x) = x^2 + bx + c, \tag{2.8}$$

$$Q = (4c - b^2)^{1/2}, \tag{2.9}$$

where density is expressed by the standard parameter r_s.

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 (2.1) and the Poisson equation (2.3) and self-consistency is attained by iteration.

III. STRUCTURE

Our system is composed of two parallel quantum wires which are coupled via thin potential barrier as is shown in Fig.1. We take the zero of the potential $V_0(\mathbf{r})$ inside of the wells and denote the height of the barrier by V_B. We may assume that the potential in the medium outside of wires has the same height V_0 as the barrier. Two quantum wires of GaAs embedded in AlGaAs may be an example of such a structure. Values for GaAs are used as the effective mass of electrons and the dielectric constant.

An appropriate set of boundary conditions for the wave function and the electrostatic potential may be the Dirichlet condition at the surface of a domain containing

our system and surrounding media with sufficient margins. In the results presented in this paper, however, we impose the Dirichlet boundary conditions for both wave functions and electrostatic potential at just outside of the region of wells and barrier. We have compared the results with the former conditions and those with the latter for a typical case to confirm that the errors due to this simplification is small (about less than 10 percent).

Since the Coulomb energy associated with the localization increases with the increase of the thickness of the barrier L_B, there may exist an upper bound for L_B to realize the localization due to the exchange and correlation effects. In this paper, we tentatively adopt a rather small value of $L_B = 17\mathring{A}$.

In applications, the external electric fields may be used to change the position of localization. The quickness of the response of our system to external fields will be limited by the quantity of charges moving to the other side when the position is reversed. In order to have a fast response, we assume that the size of wires are relatively small: In our simulation we take approximately $100\mathring{A} \times 100\mathring{A}$ wires.

The height of the barrier V_B and the total line density of electrons n_{tot} are taken as parameters and analyses will be performed for various combination of these parameters. As for doping, we assume that the electrons are introduced to our system by donors distributed in or around the wires and compare the results for two cases of their distribution.

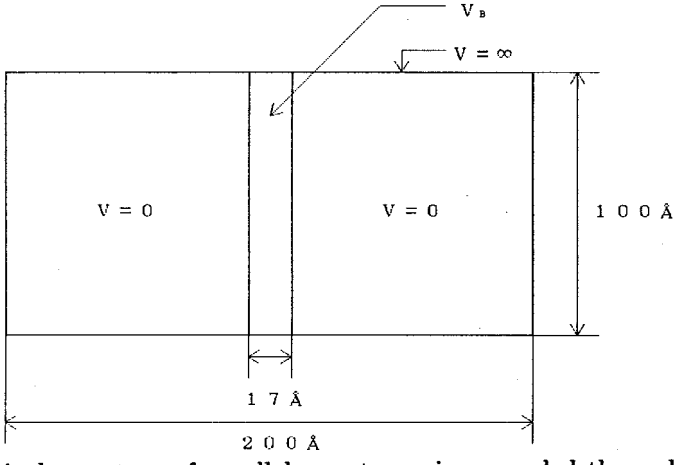

FIG. 1. Symmetrical structure of parallel quantum wires coupled through thin potential barrier. Positive charges of ionized donors are distributed with the same symmetry.

IV. RESULTS AND DISCUSSIONS

Typical examples of symmetric and asymmetric distributions are shown in Fig.2. In the asymmetric case, the reversed distribution is also possible: This bistability may be the most important point in relation to applications.

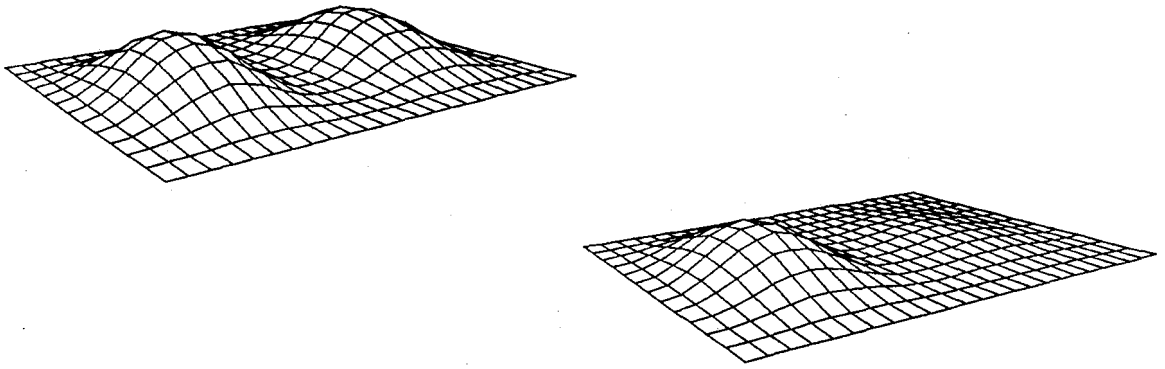

FIG. 2. Typical examples of symmetric and asymmetric electron distributions. In asymmetric case, inverted distribution has the same total energy.

A. Parameter Domain for Localization

A measure of localization may be the difference in the electron densities integrated in each well. The difference of the maximum densities in each well may also work to signal the localization. In Fig.3, we show the second measure normalized by the larger maximum density in the domain characterized by the total electron density (per unit length) n_{tot} and the barrier height V_B. In this case, the ionized donors are distributed as uniform positive charges in wells and barrier.

We observe that the localized states appears for larger values of the potential barrier height. We also note that the barrier height necessary for localization sharply increases when the total density exceeds $5 \times 10^5 \mathrm{cm}^{-1}$.

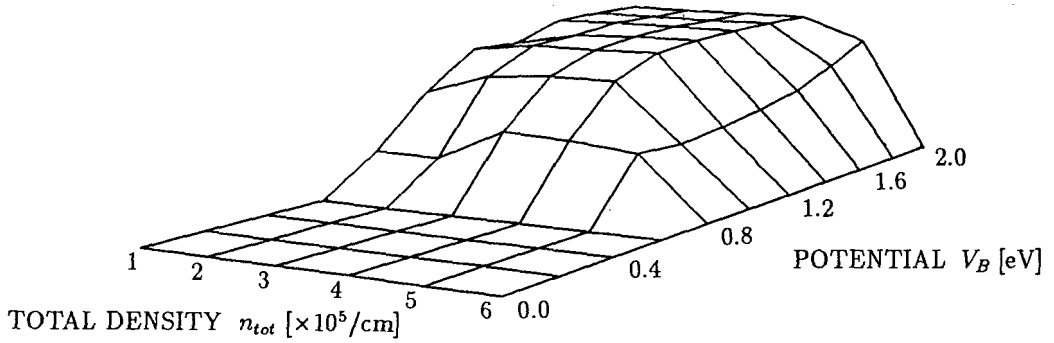

FIG. 3. Degree of localization as a function of characteristic parameters. Difference in maximum densities in each wire normalized by the lager one is shown in linear scale: Values nearly equal to 0 and 1 for smaller and larger V_B indicate symmetric and asymmetric states, respectively. Positive charge density and dielectric constant are uniform throughout the system.

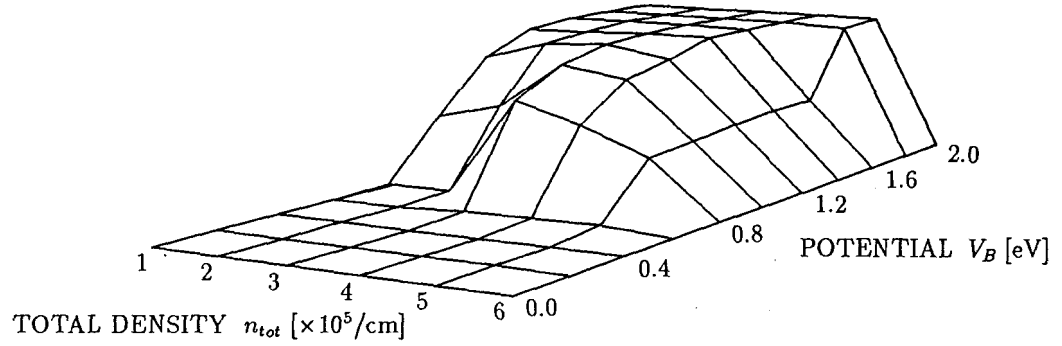

FIG. 4. The same as Fig.3. Positive charges are concentrated in the barrier.

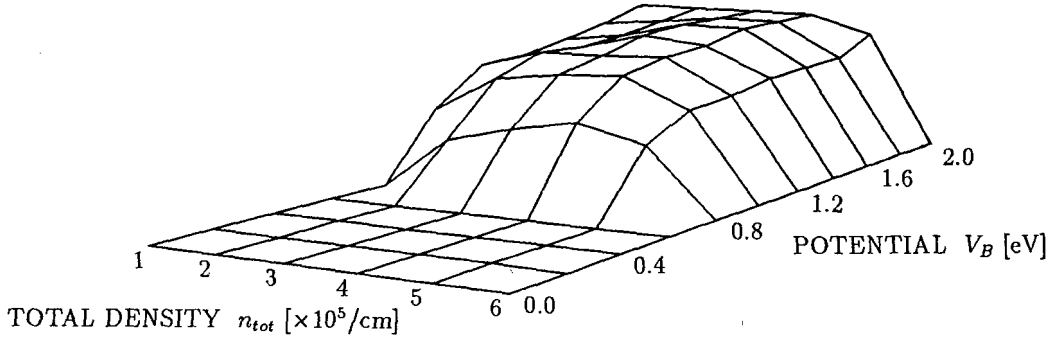

FIG. 5. The same as Fig.3. Positive charges are concentrated in the barrier and the dielectric constant there is doubled.

When Δn is the deviation of electron density in each well from symmetric distribution $n_{tot}/2$, the Hartree energy may be estimated as

$$\frac{(\Delta n)^2}{2C} \tag{4.1}$$

where the capacitance per unit length C is inversely proportional to L_B. On the other hand, the exchange-correlation energy (per unit length) may be estimated as

$$\text{const } e^2 S[(n_{tot}/2 + \Delta n)^{4/3} + (n_{tot}/2 - \Delta n)^{4/3}], \tag{4.2}$$

S being the cross section of the wire. This is proportional to

$$n_{tot}^{3/4} \left(\frac{\Delta n}{n_{tot}}\right)^2 \tag{4.3}$$

for small values of $\Delta n/n_{tot}$. We thus expect the localization for small total densities.

The potential barrier between wires will help electrons to localize. Previous results by Ruden and Wu[1, 2] correspond to the case of infinite potential.

The rapid increase of the potential height needed for localization for $n_{tot} > 5 \times 10^5 \text{cm}^{-1}$ is consistent with the above expectation. This tendency continues at larger densities not shown in Fig.3.

The critical potential height is almost independent of the total density for $n_{tot} < 4 \times 10^5 \text{cm}^{-1}$. This behavior has not been expected from the simple scaling argument. As will be shown shortly, this tendency is dependent on the distribution of positive charges and the dielectric constant and the critical value even increases in some cases. It may therefore be difficult to give a simple explanation.

B. Effect of Distribution of Positive Charges

When the positive charges are concentrated in the region between wells, the Hartree energy will be reduced in comparison with the case of uniform distribution. In Fig.4, the result in such a case is shown. We see that the critical values of the potential height for high densities are slightly reduced compared with those in Fig.3. Those for low densities, on the contrary, have the opposite tendency to our

expectation which seems to be difficult to derive intuitively. This may indicate that numerical analyses are important in this domain.

C. Effect of Distribution of Dielectric Constant

If the dielectric constant in the barrier is larger than other parts, we may again have smaller Hartree energy: the electric field between two wells is mainly responsible for the energy. The exchange correlation energy, on the other hand, will be affected to a much smaller extent.

To clarify the effect of this kind of inhomogeneity in the dielectric constant, similar computations have been performed for a system where positive charges are distributed in the barrier and the dielectric constant is doubled there. The exchange correlation energy is computed as if the barrier has the same dielectric constant as other parts. The result is shown in Fig.5.

Compared with Fig.4, the critical values of potential are reduced especially in the case of low densities. The quantitative conclusion for this effect, however, seems to be difficult to obtain. Unexpected result in the previous subsection tells us that these reductions may be fortuitous. We may rather conclude that even with inhomogeneity in dielectric constant or positive charges the results of uniform cases will be changed less than 20 percent.

V. CONCLUDING REMARKS

We have analyzed the electronic states in symmetrical quantum wires taking many-body effects into account by the density functional theory. It has been shown that electrons in such a symmetrical system have asymmetric ground states which are doubly degenerate: Electrons are mainly localized in either of wires.

The effects of distributions of positive charges and dielectric constant have also been investigated and it is shown that the general tendency of the effects are consistent with physical considerations. Quantitative conclusions, however, needs further detailed analyses.

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