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Numerical Simulation of Quantum Systems -Dynamics of Electrons in Microstructures-

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SYNOPSIS

Difficulties in simulating systems composed of classical and quantum particles lie in the treatment of the many-body interactions between quantum particles and the geometrical variety of configurations of classical particles. In order to overcome these difficulties, we have developed some numerical methods and applied them to simple cases. As for stationary states, the finite element method provides us with sufficient geometrical freedom. Combined with the Kohn-Sham equation based on the density functional theory, this method virtually satisfies our requirement. In order to investigate time-dependent phenomena, we apply the time-dependent Kohn-Sham equation. Adopting the finite difference method, we are able to follow the development of quantum many-body system. As an example, we estimate the effects of the potential height, the electric field, and many-body interactions in some transition processes in quantum wells coupled by a tunneling barrier. This example is important in itself in relation to semiconductor superlattices and also serves as a benchmark for quantum simulations, variety of geometry corresponding to that of classical particles.

1 Introduction

Numerical simulation of many-body systems is sometimes one of the most powerful approaches when we have no small parameters useful in developing

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theoretical methods. Simulations of classical systems where the interactions between particles are known have now become a kind of tool relatively easy to use owing to rapid progresses in computational hardwares. Those of systems including quantum particles, on the other hand, are still a subject of study in itself with difficulties in the treatment of the many-body interactions between quantum particles and the geometrical variety of configurations of classical particles in the system. The purpose of this paper is to develop numerical methods which overcome these difficulties.

One of useful methods which enable us to describe the electronic states in interacting systems is the density functional method. A formulation for stationary states is embodied in the Kohn-Sham equation.[1] When the time dependence is properly taken into account, we are also able to calculate the time development of many body systems by this method. In the latter case, the corresponding formulation is called the time dependent Kohn-Sham equation.[2]

As an example of application of our methods, we analyze the behavior of electrons in semiconductor superlattices. In order to apply semiconductor supperlattices to electronic devices, we need accurate analyses on electronic states in various supperlattice potentials. In simple potentials analytical solutions for one particle states are possible. In real applications, however, it is necessary to take electronic many-body interactions and geometrical effects into account and we have to resort to numerical methods even in simple cases. The geometrical variety has the same effect as the potential due to classical particles in the mixture of quantum and classical particles. This example thus serves as a test of efficiency of our methods for such mixtures.

We consider a system composed of two symmetric quantum wires coupled through a thin tunneling barrier and follow the behavior of electrons initially confined in one of the wires. Though the analysis of dynamics is naturally based on that of statics,[3] we here describe mainly time-dependent aspects of our numerical procedures.

2 Time-Dependent Kohn-Sham Equation

One can formulate the time-dependent density-functional method in the form of the time-dependent Kohn-Sham equation.[2] This formalism reduces to the following set of equations:

$$n(\mathbf{r},t) = \sum_{n}^{N} \mid \Psi_n(\mathbf{r},t) \mid^2, \tag{1}$$

$$i\hbar\frac{\partial}{\partial t}\Psi_n(\mathbf{r},t) = [-\frac{\hbar^2}{2m}\nabla^2 + v(\mathbf{r},t)]\Psi_n(\mathbf{r},t), \tag{2}$$

$$v(\mathbf{r},t) = v_{ext}(\mathbf{r},t) + e^2\int d\mathbf{r}'\frac{n(\mathbf{r}',t)}{\mid \mathbf{r}-\mathbf{r}' \mid} + \frac{\delta E_{xc}[n]}{\delta n(\mathbf{r},t)}. \tag{3}$$

Here $n(\mathbf{r},t)$, $\Psi_n(\mathbf{r},t)$, and $v_{ext}(\mathbf{r},t)$ are the electronic density, the wave function, and the external potential, respectively, and the second and the third terms on the right-hand side of (3) are the Hartree and the exchange-correlation potentials. We denote other quantities by usual symbols.

In order to make integration with respect to time, we write the approximate solution [4] first in the form

$$\begin{aligned}\Psi(\mathbf{r},t+\Delta t) &= \exp[-\frac{i\Delta t}{2\hbar}v(\mathbf{r},t+\Delta t)] \\ &\quad \exp(\frac{i\hbar\Delta t}{2m}\nabla^2)\exp[-\frac{i\Delta t}{2\hbar}v(\mathbf{r},t)]\Psi(\mathbf{r},t),\end{aligned} \tag{4}$$

and then in the form

$$\begin{aligned}\Psi(\mathbf{r},t+\Delta t) &= \exp[-\frac{i\Delta t}{2\hbar}v(\mathbf{r},t+\Delta t)] \\ &\quad (1-\frac{i\hbar\Delta t}{4m}\nabla^2)^{-1}(1+\frac{i\hbar\Delta t}{4m}\nabla^2)\exp[-\frac{i\Delta t}{2\hbar}v(\mathbf{r},t)]\Psi(\mathbf{r},t).\end{aligned} \tag{5}$$

This solution has the accuracy of the second order in time. The important points are that the operation of

$$(1-\frac{i\hbar\Delta t}{4m}\nabla^2)^{-1}(1+\frac{i\hbar\Delta t}{4m}\nabla^2) \tag{6}$$

can be performed by the Crank-Nicolson method and that the operand of this operator

$$\exp[-\frac{i\Delta t}{2\hbar}v(\mathbf{r},t)]\Psi(\mathbf{r},t) \tag{7}$$

gives the same electronic density as $\Psi(\mathbf{r},t)$ since the factor $\exp[-i\Delta t v(\mathbf{r},t)/2\hbar]$ only changes the phase of the wave function.

3 Results

3.1 Transition of Electrons in Coupled Quantum Wells

Our system is composed of two parallel quantum wires coupled by a thin potential barrier as shown Fig.1. The size of our system is taken tentatively to

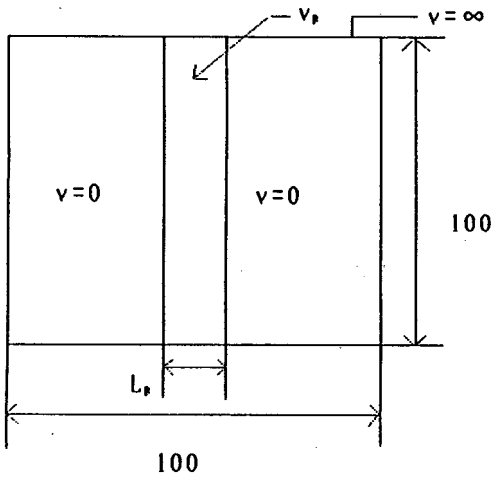

Fig.1 Structure of coupled quantum wells. Lengths are in $\mathring{A}$.

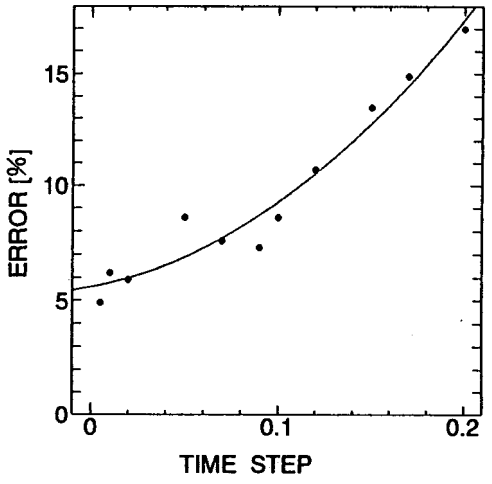

Fig.2 Relative error in time development. Time is in 0.12fs.

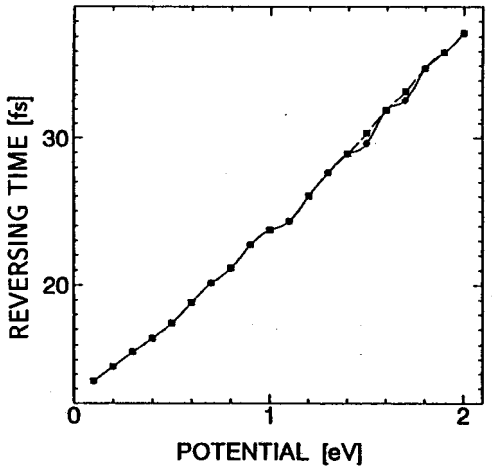

Fig.3 Time for reversing electron distribution vs. barrier height. Thickness of barrier is 12.5$\mathring{A}$.

be $100\mathring{A} \times 100\mathring{A}$. We denote the height and the thickness of the barrier by V_B and L_B, respectively. We impose the Dirichlet boundary conditions for both wave functions and the electrostatic potential at the outer boundary of the domain including wells and the barrier. We assume that electrons are in the conduction band of GaAs in the wells.

We first obtain the stationary states in our system by the finite element method and construct the initial asymmetric state for dynamic analyses by superposing the ground and the first excited states. The electronic density per length is taken to be $2 \times 10^5 \mathrm{cm}^{-1}$. Before analyzing effects of various parameters in our system, we have applied our time development scheme to the case where electrons have no interactions. In this case, the time development is completely determined by the difference in the eigenvalues of the ground and the first excited states. Comparing our numerical results with the exact results thus predicted, we have confirmed the accuracy of our procedures and determined an optimal value for the time step.

In Fig.2 we show relative errors in the time τ_{rev} needed to reverse the distribution of electrons to the other side of the barrier. We observe the increase of error for larger time steps. The behavior as a function of the time step, however, does not allow simple interpretations. Since our scheme is of the second order in the increment of time, we expect the increase of error in proportion to $(\Delta t)^2$. It is not clear whether this is confirmed. It is also inconsistent with our expectation to have a nonzero limiting value for $\Delta t \to 0$. We speculate that these unexpected behaviors may be due to insufficient spatial resolution of our analysis. We use the time step giving the error of a few percents in subsequent analyses.

The effect of the barrier height V_B on τ_{rev} is shown in Fig.3. We see that the electronic interactions have very small effect on the dependence of τ_{rev} on V_B: Irregular fluctuations from general tendency in these results seem to be due to insufficient accuracy of our method and this small effect is within these fluctuations.

The relation between the thickness of the barrier L_B and τ_{rev} is shown in Fig.4. The time τ_{rev} first increases and then decreases with the increase of the thickness: When L_B exceeds some critical value, we have no bound states in each well and τ_{rev} begins to decrease.

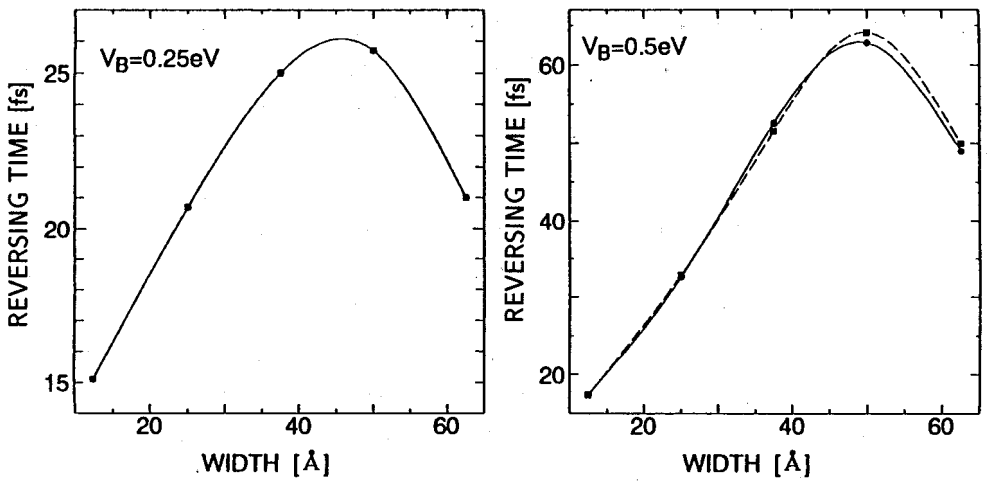

Fig.4 Time for reversing electron distribution vs. barrier thickness.

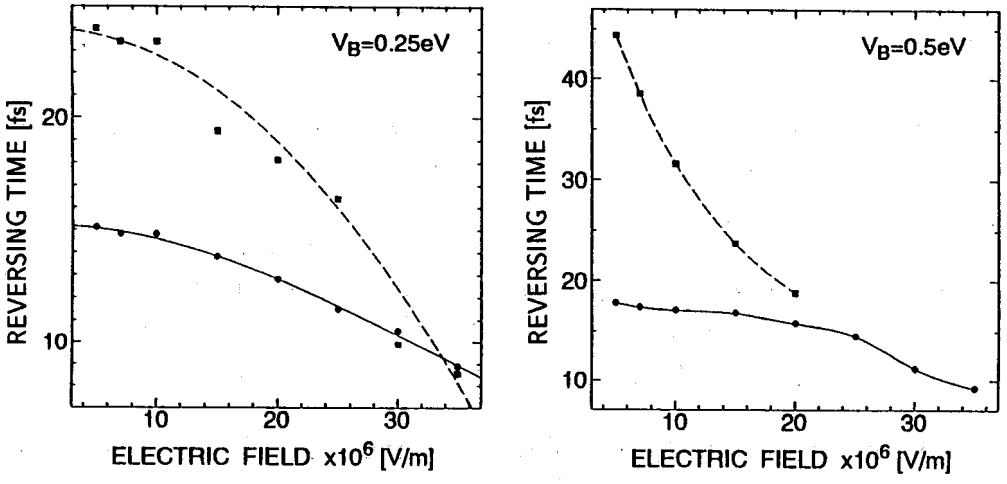

Fig.5 Time for reversing electron distribution vs. electric field. Thickness of barrier is 12.5$\AA$ (solid line) or 37.5$\AA$ (broken line).

3.2 Effect of Electric Field

Let us now examine the effect of electric field on the dynamic behavior of electrons. In Fig.5 shown are the results for four cases where the barrier height and thickness are changed. The electric field has the strength of the order of 10^7V/m. The results with or without electronic interactions give almost the same values.

The electrons move quickly when the electric fields are applied. This is intuitively natural and can be expressed in another way: Under the electric field, we have increased values for the difference of energies in the ground and the first excited states and therefore the time needed to reverse the distribution becomes short. This effect is larger for wider separation of wells as is consistent with numerical results.

4 Conclusion

We have analyzed the electronic states in symmetrical quantum wires taking many-body effects into account. Starting from the initial state obtained by the time-independent density functional theory, we have numerically followed the time development of electronic distribution based on the time dependent density functional theory.

The most interesting result may be the apparent insensitiveness of dynamical behaviors to the electronic interactions. It has been shown that they play an important role in determining stationary states in these systems[3] Therefore it seems, at least in our case, that the dynamics can be approximately described as a weakly interacting system on the basis of those eigenstates which include the many-body effects properly.

In this paper we have considered a system of electrons only in a fixed potential structure. Our method may also extended to the cases where the potential has a part due to other classical particle. A typical example of the latter may be the plasma encountered in the inertial confinement fusion.

Acknowledgements

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