Numerical study of the effect of Coulomb repulsion on resonant tunneling

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The effect of on-site Coulomb repulsion on the process of resonant tunneling is studied in the tight-binding model of a quasi-one-dimensional system. The conductance through a small region where the Coulomb interaction is strong is calculated as a function of chemical potential with use of the Kubo formula. The Green's function and the number of electrons in the region are obtained self-consistently using the recursion method in the mean-field approximation. It is found that the conductance shows various doublet structures depending on the broadening of the virtual bound state and the Coulomb interaction.

Recent advances in scanning tunneling microscopy and lithography techniques have made it possible to make various structures on the nanometer scale. These advances have brought about great interest in the possibility of realizing electron devices, where the quantum-mechanical behavior of electrons plays an essential role in their operation principles. Furthermore, in these nanometer-scale systems, the physics of electron-electron interaction has become the subject of current experimental and theoretical interest. Many experimental findings in quantum dot structures approaching atomic dimensions are reported.[1] For example, the Coulomb oscillation[2,3] and the Coulomb staircase[4] in conductance have been observed experimentally in various small dot structures, and a semiclassical stochastic model, called the Coulomb-blocade model,[5] has been significantly successful in explaining experiments on these small structures. Also, analysis of the experimental findings in view of recent numerical studies[6,7] yielded detailed information on single particle levels in the quantum dot. Thus, it is considered to be important to study the effect of Coulomb interaction on the transport phenomena from a general point of view.

At low temperatures, resonant tunneling is the dominating mechanism for particle conduction through small systems with localized states. Numerical studies for investigating the effect of intra-atomic Coulomb interaction on the resonant site in the process of resonant tunneling have been reported by several researchers. For instance, using the one-impurity Anderson model, Ng and Lee[8] reported that the resonant transmission picture of one-particle tunneling is strongly modified, and that the resulting conductance peak is expected to have a non-Lorentzian line shape due to the Kondo effect. Also, Kawabata[9] predicted, using the Friedel sum rule, in a quasi-one-dimensional system the conductance through a quantum dot is close to $2e^2/h$, if the temperature is lower than the Kondo temperature T_K.

In this study, we have calculated the conductance through a dot in the quasi-one-dimensional system numerically within the Kubo formalism using the recursion method in the case where the temperature is higher than T_K. We have obtained the Green's function and the number of electrons self-consistently in the mean-field approximation.

We consider a quasi-one-dimensional quantum wire, which is assumed to be infinitely long on either side of a small region where electrons are confined by a potential $V_{i,j,\sigma}$, as shown in Fig. 1. In order to investigate the effect of on-site Coulomb correlation on the process of resonant tunneling, we introduce the following tight-binding Hamiltonian:

$$H=t\sum_{i}\sum_{j=1}^{M-1}\sum_{\sigma}(C^{\dagger}_{i,j+1,\sigma}C_{i,j,\sigma}+C^{\dagger}_{i,j,\sigma}C_{i,j+1,\sigma})+t\sum_{i}\sum_{j=1}^{M}\sum_{\sigma}(C^{\dagger}_{i+1,j,\sigma}C_{i,j,\sigma}+C^{\dagger}_{i,j,\sigma}C_{i+1,j,\sigma})+\sum_{i}\sum_{j=1}^{M}\sum_{\sigma}\varepsilon_{i,j,\sigma}C^{\dagger}_{i,j,\sigma}C_{i,j,\sigma}$$
$$+\sum_{i=1}^{N}\sum_{j=1}^{M}\sum_{\sigma}V_{i,j,\sigma}C^{\dagger}_{i,j,\sigma}C_{i,j,\sigma}+U\sum_{i=1}^{N}\sum_{j=1}^{M}n_{i,j,\downarrow}n_{i,j,\uparrow}\,, \tag{1}$$

where $C^{\dagger}_{i,j,\alpha}$ is the creation operator with spin α at the lattice site (i,j). The quantities t (<0), $\varepsilon_{i,j,\sigma}$, and $V_{i,j,\sigma}$ are the hopping integral between the nearest neighbors, the on-site potential, and the confinement potential, respectively. The last term is an interaction term describing the effect of on-site Coulomb interaction between two electrons with different spins in region II. In the present calculations, N and M are set to 10 and 4, and $V_{i,j,\sigma}$ is

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given by

$$V_{i,j,\sigma}=\begin{cases}5|t| \text{ [at sites } (1,1),(1,M)\text{,} \\ \qquad (N,1) \text{ , and } (N,M)] \\ 0 \text{ (otherwise)} ,\end{cases} \tag{2}$$

and $\varepsilon_{i,j,\sigma}$ is zero. Next, we introduce the Green's function defined by

$$G^{\pm}[(i,j,\sigma),(i',j',\sigma'),E] \equiv \left\langle i,j,\sigma \left| \frac{1}{E-H\pm i0} \right| i',j',\sigma' \right\rangle ,$$

$$|i,j,\sigma\rangle \equiv C^{\dagger}_{i,j,\sigma}|0\rangle , \tag{3}$$

where $|0\rangle$ denotes vacuum. To calculate the Green's function corresponding to H, we employ the mean-field approximation and the recursion method[10,11] which allows us to solve for a potential of any shape. The number of electrons at the lattice site (i,j) in region II can be calculated from G^{+} by the following equation:

$$\langle n_{i,j,\alpha}\rangle = -\frac{1}{\pi}\int_{-\infty}^{\mu} dE \, \mathrm{Im}G^{+}[(i,j,\alpha),(i,j,\alpha),E] , \tag{4}$$

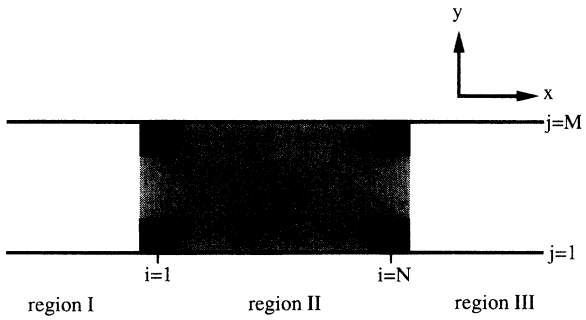

FIG. 1. Schematic illustration of the system. The closed squares express the confinement potentials. The on-site Coulomb correlation exists only in region II (shaded region). The parameters M and N are the lattice numbers for the y direction of the wire and for the x direction of region II, respectively.

where μ denotes the chemical potential. Using Eq. (4) and the recursion method, we can obtain the Green's function and the number of electrons in region II self-consistently. Then, the conductance Γ is calculated from the Green's function by making use of the Kubo formula[10,11]

$$\Gamma = \frac{2e^2t^2}{h}\sum_{j=1}^{M}\sum_{j'=1}^{M}\sum_{\sigma}\{\tilde{G}[(i,j,\sigma),(i,j',\sigma)]\tilde{G}[(i-1,j',\sigma),(i-1,j,\sigma)]$$
$$+\tilde{G}[(i-1,j,\sigma),(i-1,j',\sigma)]\tilde{G}[(i,j',\sigma),(i,j,\sigma)]$$
$$-\tilde{G}[(i,j,\sigma),(i-1,j',\sigma)]\tilde{G}[(i,j',\sigma),(i-1,j,\sigma)]$$
$$-\tilde{G}[(i-1,j,\sigma),(i,j',\sigma)]\tilde{G}[(i-1,j',\sigma),(i,j,\sigma)]\} , \tag{5}$$

with

$$\tilde{G}[(i,j,\sigma),(i',j',\sigma)] \equiv \frac{1}{2i}\{G^{-}[(i,j,\sigma),(i',j',\sigma)] - G^{+}[(i,j,\sigma),(i',j',\sigma)]\} . \tag{6}$$

Now, we discuss the electron conduction through the region where the on-site Coulomb interaction exists. For simplicity, we consider only the case where the number of propagating mode is set to unity. Figure 2 shows the conductance calculated with use of Kubo formula. For $U \le 0.5|t|$, the ground state in the present model is spin singlet with $\langle n_{i,j,\downarrow}\rangle = \langle n_{i,j,\uparrow}\rangle$. In this case, there are three conductance peaks of the resonant tunneling occurring when the chemical potential μ crosses a virtual bound state. As U increases, each position of the peak shifts to the right and the peaks are broadened [see Figs. 2(a) and 2(b)], since the levels of virtual bound state are raised by the repulsive interaction while the height of confining potential is a constant. When U is equal to $|t|$, the first peak of the conductance splits into two [see Fig. 2(c)]; each peak corresponds to the process of the resonant tunneling for electrons with up or down spin. The solution of $\langle n_{\downarrow}\rangle \neq \langle n_{\uparrow}\rangle$ can appear in the condition[12] of

$$\frac{U}{\Delta} \ge \frac{\pi}{\sin^2\pi\langle n\rangle} , \tag{7}$$

where Δ is the resonance half-width and $\langle n\rangle$ is the total number of electrons in the virtual bound state. For $U \ge 5|t|$, the condition of Eq. (7) can be satisfied for all virtual bound states, and hence, one can notice the doublet structure for every conductance peak [see Figs. 3(a) and 4(a)]. For $U \ge 5|t|$, the third peak in the case at $U=0$ shifts to the region for $\mu \ge |t|$. To clarify the behavior of electrons with up and down spins, we have calculated the number of electrons in region II as a function of μ. First, we consider the case of $U=5|t|$. As can be seen from Fig. 3(b), when μ is much smaller than the value of the lowest virtual bound state, the distribution of up-spin electrons is identical with that of down-spin electrons. When μ approaches the virtual bound state, the number of electrons with up spin increases while that with down spin decreases, since the condition of Eq. (7) can be satisfied. When μ passes through the virtual bound state with down-spin electrons, the ground state becomes spin singlet again. This is because repulsive interaction between electrons is no longer significant, in the

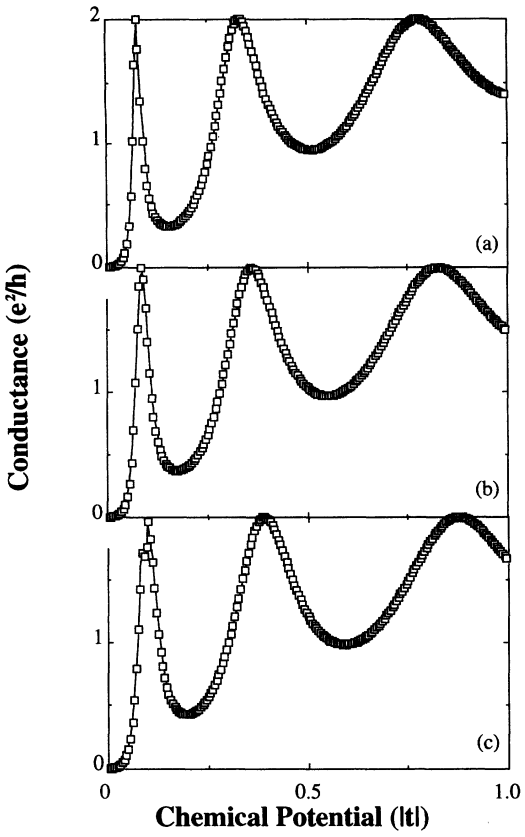

FIG. 2. Conductance plotted as a function of μ. Chemical potential is measured from the energy of the bottom of the lowest subband. The magnitude of U is (a) 0, (b) $0.5|t|$, and (c) $|t|$.

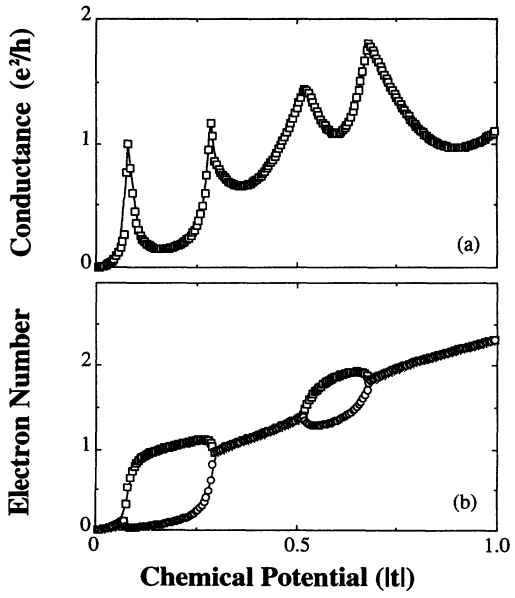

FIG. 3. (a) Conductance plotted as a function of μ. The magnitude of U is $5|t|$. (b) The number of electrons plotted as a function of μ. The circles and the squares denote the up-electron number and the down-electron number in the region II.

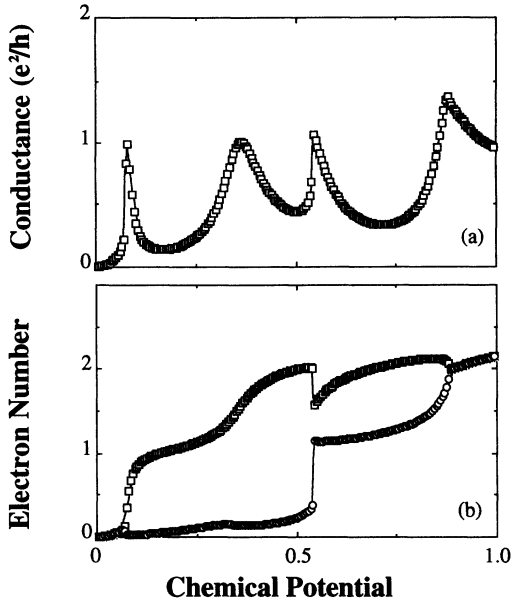

FIG. 4. (a) Conductance plotted as a function of μ. The magnitude of U is $7|t|$. (b) The number of electrons plotted as a function of μ. The circles and the squares denote the up-electron number and the down-electron number in the region II.

case where there are the same number of levels for up- and down-spin electrons below μ. The features of spin split of virtual bound states, which depend on U, are schematically shown in Fig. 5(b). Thus, at $U=5|t|$, levels for up and down spins appear alternately, and in principle, the aspects in Fig. 3 are considered to be analogous to those predicted qualitatively by Kawabata.[9] Next, the case of $U=7|t|$ is considered. In this case, the second level for up spin comes to be lower than the first level for down spin [see Fig. 5(c)], and hence, magnetic transition with spin rearrangement takes place at the second level for up spin, as shown in Fig. 4. Thus, resonances for electrons on the same spins occur successively, and in most region of μ, the solution of $\langle n_\downarrow \rangle \neq \langle n_\uparrow \rangle$ appears (see Fig. 4).

In the present calculations, we did not consider the electrostatic energy e^2/C,[2] where C is the capacitance between dot and lead, so that the period of the successive resonance peaks cannot be compared with that in the ex-

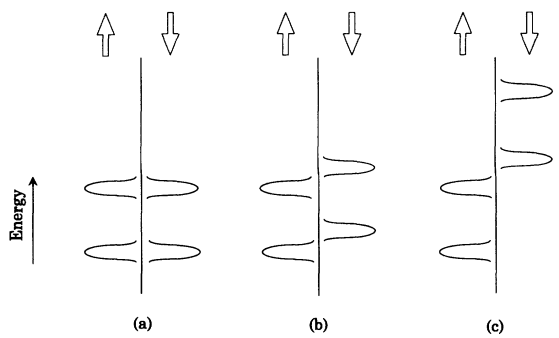

FIG. 5. Schematic figures of the virtual bound states depending on U. (a) $U=0$, (b) $U=5|t|$, and (c) $U=7|t|$.

periment of the Coulomb oscillation. Moreover, our calculation is based on the mean-field approximation so that, of course, we can hardly comment on the Kondo problem. However, as is shown so far, by our method we can investigate the electronic properties of the dot which have a structure spread over many sites. Also, we will study the effect of disorder and constriction geometry on the electron transport through the region where the Coulomb interaction is strong in the near future.

In conclusion, we have calculated the conductance and electronic state in a quantum wire with confinement potentials self-consistently. We have investigated the effect of on-site Coulomb correlation on the process of resonant tunneling. It has been found that the conductance shows various doublet structures depending on the height and broadening of the virtual bound state and the Coulomb interaction. Our method can also be applied to multimode quantum wire, and those results will be given elsewhere.

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[1]For a review, see H. van Houten, C. W. J. Beenakker, and A. A. M. Staring, in *Single Charge Tunneling,* Vol. 294 of *NATO Advanced Study Institute, Series B: Physics,* edited by H. Grabert and M. H. Devoret (Plenum, New York, 1992).

[2]U. Meirav, M. A. Kastner, and S. J. Wind, Phys. Rev. Lett. **65**, 771 (1990).

[3]L. McEuen, E. B. Fovman, U. Meirav, M. A. Kastner, Y. Meir, and N. S. Wingreen, Phys. Rev. Lett. **66**, 1926 (1991).

[4]J. B. Barner and S. T. Ruggiero, Phys. Rev. Lett. **59**, 807 (1987).

[5]D. V. Averin and K. K. Likharev, in *Mesoscopic Phenomena in Solides,* edited by B. L. Altshuler, P. A. Lee, and R. A. Webb (Elsevier, Amsterdam, 1991).

[6]Y. Meir, N. S. Wingreen, and P. A. Lee, Phys. Rev. Lett. **66**, 3048 (1991).

[7]C. W. J. Beenakker, Phys. Rev. B **44**, 1646 (1991).

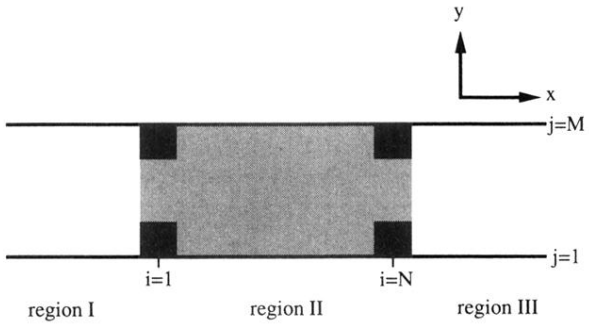
[8]T. K. Ng and P. A. Lee, Phys. Rev. Lett. **61**, 1768 (1988).

[9]A. Kawabata, J. Phys. Soc. Jpn. **60**, 3222 (1991).

[10]P. A. Lee and D. S. Fisher, Phys. Rev. Lett. **47**, 882 (1981).

[11]Y. Asano, A. Oguri, and S. Maekawa, Phys. Rev. B **48**, 6192 (1993).

[12]P. W. Anderson, Phys. Rev. **124**, 41 (1961).



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