Electron transport through a double-quantum-dot structure with intradot and interdot Coulomb interactions

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(Received 24 May 1999)

Electron transport through a double-quantum-dot structure with intradot and interdot Coulomb interactions is studied by a Green's function (GF) approach. The conductance is calculated by a Landauer-Büttiker formula for the interacting systems derived using the nonequilibrium Keldysh formalism and the GF's are solved by the equation-of-motion method. It is shown that the interdot-coupling dependence of the conductance peak splitting matches the recent experimental observations. Also, the breaking of the electron-hole symmetry is numerically demonstrated by the presence of the interdot repulsion. [S0163-1829(99)01640-9]

Advances in nanotechnologies have made it feasible to fabricate quantum-dot (QD) structures with electronic confinement approaching atomic dimensions. Because the Coulomb repulsion within the dot is important, it is suggested[1–4] that the tunneling through the QD and the main correlation effects associated with the QD can be appropriately described by the Anderson model. Recently, transport properties of the double QD structures have received much attention, both experimentally[5,6] and theoretically.[7–9] As a direct extension of the single-dot system, the double QD structure consists of two coupled QD's, of which each dot is connected to a lead by a tunnel barrier. The experimental measurements[5] demonstrated that as the interdot coupling increases, the conductance peaks are split into two peaks each and the peak splitting increases with the interdot coupling. Very recently, Oosterkamp *et al.*[10] and Blick *et al.*[11] performed experimental measurements on the true tunnel splitting of the double QD and explicitly demonstrated the formation of artificial molecular states in the strong interdot coupling regime. In the theoretical aspect, the many-body eigenstates are calculated by direct diagonalization of the Hamiltonian for the isolated double QD and the effect of the leads is incorporated through a rate equation.[7,8] Because the leads are neglected in calculating the many-body eigenstates of the double QD structure, this approach, as noted in Ref. 7, is valid only when the lead coupling is small enough.

In the present paper, we study the transport properties of the double QD structure by employing an Anderson-type model that includes both intradot and interdot Coulomb interactions. In contrast with previous works,[7,8] our approach takes the lead coupling into account and treats the total Hamiltonian as a whole in calculating the spectral properties of the double QD system. The conductance is calculated by a Landauer-Büttiker formula for the interacting systems, which is derived using the nonequilibrium Keldysh formalism. The causal Green's functions (GF's) used in the calculations are solved by the equation-of-motion method.

The Hamiltonian we study is an Anderson-type model in the tight-binding representation:

$$H = H_d + H_t + H_0, \tag{1}$$

with

$$H_d = \sum_{\sigma} \left[E_A c_{A\sigma}^{\dagger} c_{A\sigma} + E_B c_{B\sigma}^{\dagger} c_{B\sigma} + T_{AB} (c_{A\sigma}^{\dagger} c_{B\sigma} + \text{H.c.}) \right] + U_A n_{A\uparrow} n_{A\downarrow} + U_B n_{B\uparrow} n_{B\downarrow} + V_{AB} \sum_{\sigma\sigma'} n_{A\sigma} n_{B\sigma'}, \tag{2}$$

$$H_t = T_L \sum_{\sigma} (c_{A\sigma}^{\dagger} c_{\alpha\sigma} + \text{H.c.}) + T_R \sum_{\sigma} (c_{B\sigma}^{\dagger} c_{\beta\sigma} + \text{H.c.}), \tag{3}$$

and

$$H_0 = \sum_{i,\sigma} \left[\varepsilon_i c_{i\sigma}^{\dagger} c_{i\sigma} + t_l (c_{i\sigma}^{\dagger} c_{i-1,\sigma} + \text{H.c.}) \right] + \sum_{j,\sigma} \left[\varepsilon_j c_{j\sigma}^{\dagger} c_{j\sigma} + t_r (c_{j\sigma}^{\dagger} c_{j+1,\sigma} + \text{H.c.}) \right]. \tag{4}$$

Here, H_d is the Hamiltonian of an isolated double QD, in which $n_{A\sigma}$ ($n_{B\sigma}$) is the number operator for electrons with spin σ in dot A (B). The term $U_A n_{A\uparrow} n_{A\downarrow}$ ($U_B n_{B\uparrow} n_{B\downarrow}$) in Eq. (2) characterizes the effect of Coulomb interaction between two electrons of different spins in dot A (B), while the last term in Eq. (2) characterizes the effect of interdot Coulomb interaction. In the double-QD structure, U_A and U_B are typically much larger than the interdot repulsion V_{AB} and the transfer integrals $|T_L|$, $|T_R|$, and $|T_{AB}|$. The Hamiltonian H_t describes the transfers of electrons between the left lead and dot A, and between the right lead and dot B. Equation (4) gives the Hamiltonian of the left and right leads, where $\varepsilon_i = \varepsilon_\alpha$ for $i = \alpha$ (the rightmost site of the left lead) and $\varepsilon_i = \varepsilon_l$ for sites $i = -1, -2, -3, \ldots$, while $\varepsilon_j = \varepsilon_\beta$ for $j = \beta$ (the leftmost site of the right lead) and $\varepsilon_j = \varepsilon_r$ for sites $j = 1,2,3, \ldots$.

Following Caroli *et al.*,[12] by means of the Keldysh formalism[13] for nonequilibrium systems, the total current through the double QD can be expressed as the sum of elastic and inelastic contributions. In the linear-response regime, it can be derived that the total conductance is given by

$$\mathcal{G} = \mathcal{G}_{\text{el}} + \mathcal{G}_{\text{inel}},$$

$$\mathcal{G}_{\rm el}=\frac{e^2}{h}\sum_\sigma \int dE\left(-\frac{\partial f(E)}{\partial E}\right)\mathcal{T}_\sigma^{\rm el}(E),$$

$$\mathcal{G}_{\rm inel}=\frac{e^2}{h}\sum_\sigma \int dE\left(-\frac{\partial f(E)}{\partial E}\right)\mathcal{T}_\sigma^{\rm inel}(E). \tag{5}$$

Here, $\mathcal{G}_{\rm el}$ and $\mathcal{G}_{\rm inel}$ involve the elastic and inelastic processes, $f(E)$ is the Fermi-Dirac distribution, and $\mathcal{T}_\sigma^{\rm el}(E)$ and $\mathcal{T}_\sigma^{\rm inel}(E)$ are

$$\mathcal{T}_\sigma^{\rm el}(E)=4\pi^2T_L^2T_R^2|G_{AB\sigma}^r(E)|^2\rho_{\alpha\sigma}(E)\rho_{\beta\sigma}(E),$$

$$\mathcal{T}_\sigma^{\rm inel}(E)=4\pi T_L^2\rho_{\alpha\sigma}(E)[|G_{AA\sigma}^r(E)|^2\{-{\rm Im}(\Sigma_{A\sigma})\}+|G_{AB\sigma}^r(E)|^2\{-{\rm Im}(\Sigma_{B\sigma})\}], \tag{6}$$

where $\rho_{\alpha\sigma}(E)$ and $\rho_{\beta\sigma}(E)$ are the local densities of states (LDOS's) on sites α and β in the isolated left and right leads, and $G_{AA\sigma}^r(E)$ and $G_{AB\sigma}^r(E)$ are Fourier transforms of the retarded GF's

$$G_{AA\sigma}^r(t)=-\frac{i}{\hbar}\theta(t)\langle\{c_{A\sigma}(t),c_{A\sigma}^\dagger(0)\}\rangle,$$

$$G_{AB\sigma}^r(t)=-\frac{i}{\hbar}\theta(t)\langle\{c_{A\sigma}(t),c_{B\sigma}^\dagger(0)\}\rangle. \tag{7}$$

Alternatively, the total conductance (5) can be rewritten as

$$\mathcal{G}=\frac{e^2}{h}\sum_\sigma \int dE\left(-\frac{\partial f(E)}{\partial E}\right)\mathcal{T}_\sigma(E), \tag{8}$$

with $\mathcal{T}_\sigma(E)=\mathcal{T}_\sigma^{\rm el}(E)+\mathcal{T}_\sigma^{\rm inel}(E)$. Apparently, it is a Landauer-Büttiker-type formula[14] generalized to the interacting systems.

The causal GF's given in Eq. (6) are here solved by the equation-of-motion technique.[15,16] Employing a decoupling procedure similar to that for the Hubbard model,[17] we obtain the explicit expressions for $G_{AA\sigma}^r(E)$ and $G_{AB\sigma}^r(E)$

$$G_{AA\sigma}^r(E)=\frac{G_{A\sigma}^{(0)}}{1-G_{A\sigma}^{(0)}G_{B\sigma}^{(0)}T_{AB}^2},$$

$$G_{AB\sigma}^r(E)=\frac{G_{A\sigma}^{(0)}G_{B\sigma}^{(0)}T_{AB}}{1-G_{A\sigma}^{(0)}G_{B\sigma}^{(0)}T_{AB}^2}, \tag{9}$$

where

$$G_{A\sigma}^{(0)}(E)=\frac{g_{A\sigma}}{1-g_{A\sigma}T_L^2/(Z-\varepsilon_\alpha^*)},$$

$$G_{B\sigma}^{(0)}(E)=\frac{g_{B\sigma}}{1-g_{B\sigma}T_R^2/(Z-\varepsilon_\beta^*)}, \tag{10}$$

with $Z=E+i\eta$, in which $\eta\to 0$. Here, the renormalized site energies ε_α^* and ε_β^* are derived by the real-space renormalization-group method,[18,19] which correspond to the fixed points of the renormalization-group equations

$$t_i'=\frac{t_i^2}{Z-\varepsilon_i},\quad \varepsilon_i'=\varepsilon_i+2t_i',\quad \varepsilon_j'=\varepsilon_j+t_i', \tag{11}$$

with $i=l$ for $j=\alpha$ and $i=r$ for $j=\beta$, while $g_{A\sigma}(Z)$ and $g_{B\sigma}(Z)$ are given by

$$g_{A\sigma}(Z)=g_{A\sigma}^{(0)}(Z)+\frac{V_{AB}}{Z-E_A}\left[g_{A\sigma}^{(1)}(Z)+g_{A\sigma}^{(2)}(Z)+\frac{U_A}{Z-E_A-U_A}g_{A\sigma}^{(3)}(Z)\right], \tag{12}$$

$$g_{B\sigma}(Z)=g_{B\sigma}^{(0)}(Z)+\frac{V_{BA}}{Z-E_B}\left[g_{B\sigma}^{(1)}(Z)+g_{B\sigma}^{(2)}(Z)+\frac{U_B}{Z-E_B-U_B}g_{B\sigma}^{(3)}(Z)\right]. \tag{13}$$

In Eq. (12), $g_{A\sigma}^{(i)}(Z)$, $i=0,1,2$, and 3, are given by

$$g_{A\sigma}^{(0)}(Z)=\frac{1-\langle n_{A\bar\sigma}\rangle}{Z-E_A}+\frac{\langle n_{A\bar\sigma}\rangle}{Z-E_A-U_A}. \tag{14}$$

$$g_{A\sigma}^{(1)}(Z)=\frac{(1-\langle n_{A\bar\sigma}\rangle)\langle n_{B\sigma}\rangle}{Z-E_A-V_{AB}(1+\langle n_{B\bar\sigma}\rangle)}+\frac{\langle n_{A\bar\sigma}\rangle\langle n_{B\sigma}\rangle}{Z-E_A-U_A-V_{AB}(1+\langle n_{B\bar\sigma}\rangle)}, \tag{15}$$

$$g_{A\sigma}^{(2)}(Z)=\frac{(1-\langle n_{A\bar\sigma}\rangle)\langle n_{B\bar\sigma}\rangle}{Z-E_A-V_{AB}(1+\langle n_{B\sigma}\rangle)}+\frac{\langle n_{A\bar\sigma}\rangle\langle n_{B\bar\sigma}\rangle}{Z-E_A-U_A-V_{AB}(1+\langle n_{B\sigma}\rangle)}, \tag{16}$$

$$g_{A\sigma}^{(3)}(Z)=\frac{\langle n_{A\bar\sigma}\rangle\langle n_{B\sigma}\rangle}{Z-E_A-U_A-V_{AB}(1+\langle n_{B\bar\sigma}\rangle)}+\frac{\langle n_{A\bar\sigma}\rangle\langle n_{B\bar\sigma}\rangle}{Z-E_A-U_A-V_{AB}(1+\langle n_{B\sigma}\rangle)}. \tag{17}$$

As for Eq. (13), there is $V_{BA}=V_{AB}$ and $g_{B\sigma}^{(i)}(Z)$, $i=0,1,2$, and 3, are obtained from Eqs. (14)-(17) by replacing A (B) with B (A). A similar decoupling procedure was also employed in Ref. 1 to derive the retarded GF of a single QD structure, which is valid for temperatures higher than the Kondo temperature.[16]

To calculate the causal GF's, one needs to obtain the average occupation numbers in dots A and B

$$\langle n_{i\sigma}\rangle=\langle c_{i\sigma}^\dagger c_{i\sigma}\rangle=\int dE f(E)\left(-\frac{1}{\pi}{\rm Im}[G_{ii\sigma}^r(E)]\right),\quad i=A,B. \tag{18}$$

Since the retarded GF's $G_{AA\sigma}^r(E)$ and $G_{BB\sigma}^r(E)$ depend on $\langle n_{A\bar\sigma}\rangle$ and $\langle n_{B\bar\sigma}\rangle$ through $g_{A\sigma}(Z)$ and $g_{B\sigma}(Z)$, the average occupation numbers $\langle n_{A\sigma}\rangle$ and $\langle n_{B\sigma}\rangle$ are thus determined self-consistently. Also, it can be derived that the selfenergies $\Sigma_{A\sigma}$ and $\Sigma_{B\sigma}$ in Eq. (6) are given by

$$\Sigma_{A\sigma}=Z-E_A-U_A\langle n_{A\bar\sigma}\rangle-V_{AB}(\langle n_{B\sigma}\rangle+\langle n_{B\bar\sigma}\rangle)-1/g_{A\sigma}(Z),$$

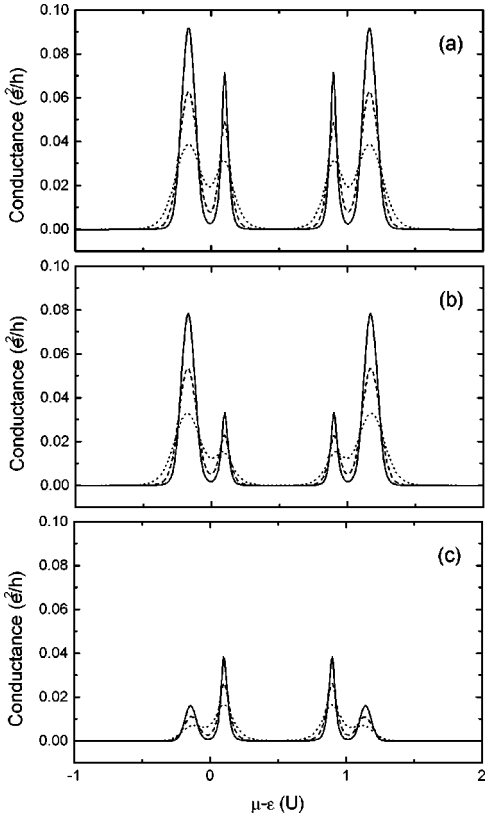

FIG. 1. (a) Total, (b) elastic, and (c) inelastic conductances, $\mathcal{G}$, $\mathcal{G}_{\rm el}$, and $\mathcal{G}_{\rm inel}$, as a function of $\mu-\varepsilon$, where $t=-0.1U$, $T_{AB}=-0.2U$, $V_{AB}=0$, and $k_BT/U=0.02$, 0.03, and 0.05 for solid, dashed and dotted curves. In this figure and the following ones, $\varepsilon_l=\varepsilon_r=\varepsilon_\alpha=\varepsilon_\beta=0$, and $t_l=t_r=-5U$.

$$\Sigma_{B\sigma}=Z-E_B-U_B\langle n_{B\bar{\sigma}}\rangle-V_{AB}(\langle n_{A\sigma}\rangle+\langle n_{A\bar{\sigma}}\rangle)-1/g_{B\sigma}(Z), \tag{19}$$

and the LDOS's $\rho_{\alpha\sigma}(E)$ and $\rho_{\beta\sigma}(E)$ are

$$\rho_{i\sigma}(E)=-\frac{1}{\pi}\mathrm{Im}\left(\frac{1}{Z-\varepsilon_i^*}\right),\quad i=\alpha,\beta. \tag{20}$$

In terms of the retarded GF's (9), the self-energies (19), and the LDOS's (20), one can numerically calculate the conductance through the double QD structure.

In the following, we present numerical calculations for the conductance. As a typical example, we study the symmetric double QD structure with parameters: $E_A=E_B=\varepsilon$, $U_A=U_B=U$, $T_L=T_R=t$, $\varepsilon_l=\varepsilon_r=\varepsilon_\alpha=\varepsilon_\beta=0$, and $t_l=t_r=-5U$. Here, the nonmagnetic case is considered, in which $\langle n_{A\uparrow}\rangle=\langle n_{A\downarrow}\rangle$ and $\langle n_{B\uparrow}\rangle=\langle n_{B\downarrow}\rangle$. First, we start with the case of zero interdot repulsion $V_{AB}=0$. This situation is suitable to the commonly-used lateral QD structures, since the interdot Coulomb repulsion is greatly reduced by the gates placed close to the dots.[7] In Fig. 1, we display the total, elastic and inelastic conductances, $\mathcal{G}$, $\mathcal{G}_{\rm el}$ and $\mathcal{G}_{\rm inel}$, as a function of $\mu-\varepsilon$, where μ is the chemical potential. The temperatures are $k_BT/U=0.02$, 0.03 and 0.05 for solid, dashed, and dotted curves, and other parameters are chosen to be $t=-0.1U$ and $T_{AB}=-0.2U$. On increasing the temperature, every two strongly-split peaks around ε and $\varepsilon+U$ decrease in peak heights and increase in peak widths, analogous to that of a noninteracting, single-particle resonance. Interestingly, in every two split peaks in the total conductance, the higher peak is mainly contributed by the conductance resonance involving elastic process, while the contribution to the lower peak by the resonance involving inelastic process is comparable to the elastic one. Recently, Chen *et al.*[7] and Klimeck *et al.*[8] obtained numerical results similar to Fig. 1(a). In their calculations, the QD array is decoupled from the leads and its many-body eigenstates are derived by direct diagonalization of the Hamiltonian for the isolated QD array. As noted by them,[7] this approach is valid only when the lead coupling is small so that the modification of the QD eigenstates may be ignored. However, in our approach, the lead coupling is taken into account and the total Hamiltonian (1) is treated as a whole in studying the spectral properties.

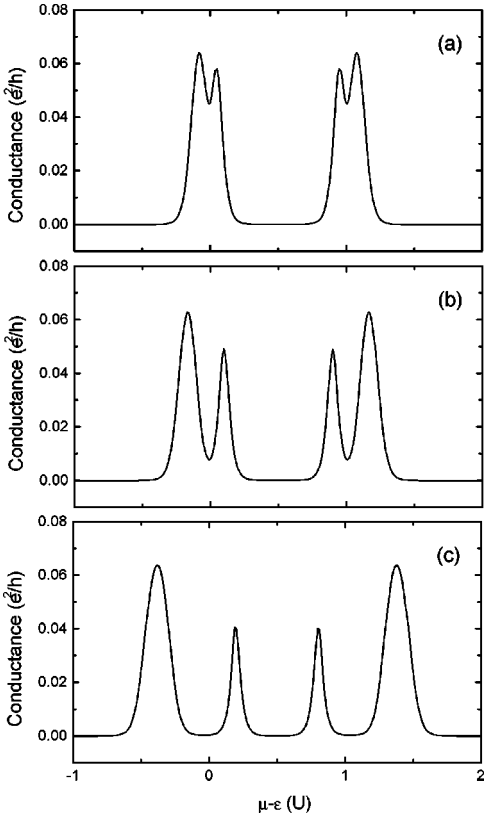

FIG. 2. Change of the conductance $\mathcal{G}$ with interdot coupling T_{AB}, where $t=-0.1U$, $V_{AB}=0$, $k_BT=0.03U$, and $T_{AB}/U=$ (a) -0.1, (b) -0.2, and (c) -0.45.

Figure 2 demonstrates the change of the conductance $\mathcal{G}$ with increasing interdot coupling T_{AB}. For weak-interdot coupling, the conductance consists of weakly split peaks [see Fig. 2(a)]. As the interdot coupling further decreases, the two split peaks are not resolved; analogous to the single-dot structure,[1] the conductance exhibits peaks at ε and $\varepsilon+U$ instead. On the contrary, corresponding to the situation that the artificial molecular states are well formed in the double QD, clearly split peaks are observed at larger values of the interdot coupling and the peak splitting widens with increasing interdot coupling. In Fig. 2(c), the conductance becomes to have four peaks with nearly equal spacing, implying that the interdot coupling is so strong that the two coupled dots are combined to become a single-large dot. These observations match the experimental measurements on the conductance of a lateral double QD structure.[5] Very recently,

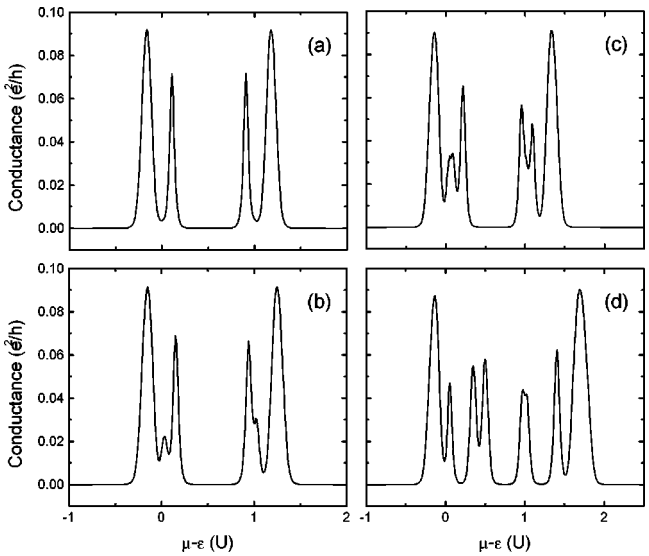

FIG. 3. Change of the conductance $\mathcal{G}$ with interdot Coulomb repulsion V_{AB}, where $t=-0.1U$, $T_{AB}=-0.2U$, $k_BT=0.02U$, and $V_{AB}/U=$ (a) 0.01, (b) 0.05, (c) 0.1, and (d) 0.3.

Oosterkamp *et al.*[10] reported a transition from ionic bonding to covalent bonding in a double QD, as probed by microwave excitations, and Blick *et al.*[11] demonstrated the tunnel-splitting effects of the double QD by measuring the charging diagrams and the differential conductance. As expected, these experiments explicitly reveal that, in the presence of strong-interdot couplings, the artificial molecular states are well formed in the double QD.

In Fig. 3, we show the change of the conductance by varying the interdot Coulomb repulsion. With increasing interdot repulsion, new resonance peaks appear. At $V_{AB}=0.05U$, three resonance peaks are resolved in both the upper and lower groups of the conductance [see Fig. 3(b)]. For $V_{AB}=0.1U$, three resonance peaks are well resolved in the upper group and four peaks start to be resolved in the lower group [see Fig. 3(c)]. Furthermore, with the interdot repulsion increased to $V_{AB}=0.3U$, four resonance peaks start to be resolved in the upper group of the conductance, while the four peaks in the lower group are clearly demonstrated [see Fig. 3(d)]; when the interdot repulsion is further increased, all of the four peaks are well resolved in both the upper and lower groups of the conductance. In the absence of the interdot repulsion, the upper and lower groups of the conductance are symmetric about $\mu-\varepsilon=0.5U$, due to the electron-hole symmetry[7] (see also Figs. 1 and 2). However, with the interdot repulsion introduced, the conductance spectrum broadens and the upper and lower groups become asymmetric (see Fig. 3). As explained by Chen *et al.*[7] this is due to the breaking of the electron-hole symmetry by the presence of the interdot repulsion.

In conclusion, we have studied electron transport through a double-QD structure with intradot and interdot Coulomb interactions. The conductance is calculated by a Landauer-Büttiker formula for the interacting systems and the causal GF's are solved by the equation-of-motion method. The Landauer-Büttiker formula is derived using the nonequilibrium Keldysh formalism, in which both the elastic and inelastic contributions are included. We show the interdot-coupling dependence of the peak splitting, which agrees with the experimental observations on double-dot conductance. Also, the breaking of the electron-hole symmetry is numerically demonstrated by introducing the interdot Coulomb repulsion.

This work was supported by the National Natural Science Foundation of China, the National Climbing Program of China, and the Chinese Academy of Sciences. One of the authors (J.Q.Y.) was also supported by the K. C. Wong Education Foundation, Hong Kong.

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