Aperiodicity-induced effects on the transmission resonances in multibarrier systems

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Abstract. We study the resonant tunneling properties of an electron through a few types of binary periodic and aperiodic multibarrier systems. Within the framework of the effective-mass approximation, we calculate the transmission coefficients to investigate the dependence of the transmission resonances on the system parameters such as the kind of aperiodicity, the generation number, and the widths of the wells and barriers. Similarities and differences of the resonances between the binary periodic and aperiodic systems are discussed in detail. Transmission resonances in aperiodic systems are found to be characterized by complex resonance splitting and a variety of peak-to-valley ratios which are not exhibited in the periodic system. For some energy ranges, transmission resonances in aperiodic systems are also found to resemble those in the periodic system, despite the existence of aperiodicity.

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1 Introduction

Tunneling of an electron through a potential barrier is one of the fundamental phenomena in quantum mechanics and plays a key role in the physics of electronic and optoelectronic devices [1]. Stimulated by the advancement in modern material fabrication technology such as molecular-beam epitaxy and metal-organic chemical vapor deposition, there has been a lot of work on the problem of the electronic resonant tunneling in semiconductor superlattices [2-15]. Among interesting features emerged from the studies, the most well recognized features are the resonance splitting effects and the energy band effects; for a finite superlattice composed of \( N \) identical potential barriers with arbitrary profiles at zero bias, there occurs
(N − 1)-fold resonance splitting, and the split resonant energies approach the band structure for large N [1, 12-14]. Very recently, Guo et al. [15] studied the resonance splitting effects in superlattices which are periodically juxtaposed with two different building barriers to demonstrate that the resonance splitting is determined not only by the structure but also by the parameters of building barriers.

In a different context, there has been much interest in the electronic properties of deterministic aperiodic systems [16-19] which are known to have more complex geometrical structures than the periodic system. Studies on these systems have revealed a variety of exotic electronic properties such as the singular continuity of the energy spectrum, the self-similarity of the electronic wave functions, the power-law behavior of the resistance, and so forth. However, most of the work has focused on the electronic properties in the infinite limit of the system size [16-20], and the study on the transport properties of the finite-size systems, particularly from tunneling point of view, has received less attention. Recently, Singh et al. [21] studied the electronic transport properties of the Fibonacci and Thue-Morse (TM) superlattices to compare the results with those of the periodic system. Besides, Liu et al. [22] calculated the electronic transmission spectra of the Cantor fractal multibarrier systems to show that the tunneling spectrum is more complex than that of the periodic system.

In this paper, we study the aperiodicity-induced effects on the transmission resonances in a few types of binary aperiodic multibarrier systems. To do this, taking into account four kinds of binary multibarrier systems whose geometrical structures are determined by Eq. (11), we calculate the transmission coefficients of an electron through these multibarrier systems. Dependence of the transmission resonances on the system parameters such as the kind of aperiodicity, the generation number, and the widths of the wells and barriers is investigated. From this, we first illustrate the characteristics of the transmission resonances exhibited in the binary periodic (BP) system, and then make a comparison of the resonances between the BP and aperiodic systems; similarities and differences between them are presented in detail. In doing this, a comparison of the resonance splitting exhibited in the common-well (CW) structure with those exhibited in the common-barrier (CB) structure of the systems is also presented.

2 Method

We shall now derive an expression for the transmission coefficient of a multibarrier system using the transfer matrix formalism. To do this, we consider an electron with a longitudinal energy $E$ incident from left of the system. As-
assuming that the phonon scattering can be neglected and no bias is applied across the system, the effective-mass approximation leads to the continuous Schrödinger equation

\[-\frac{\hbar^2}{2m^*_j} \frac{d^2}{dx^2} + V(x) \psi_j(x) = E \psi_j(x),\]

where \( x \) is the longitudinal direction of the system, \( V(x) \) the minimum energy of the conduction band, and \( m^*_j = m^*_{w(b)} \) the effective mass of the electron in the well (barrier) of the \( j \)th cell. Figure 1 shows the schematic configuration of a part of the system. For convenience of calculation, we set the conduction band minimum to be zero and the potential barrier to be rectangular, i.e.,

\[ V(x) = \begin{cases} 0 & \text{for } x_j < x < y_j \\ V & \text{for } y_j < x < x_{j+1} \end{cases}, \]

where \( x_j (y_j) \) is the starting position of the \( j \)th well (barrier). Then, the wave function associated with the electron in the \( j \)th cell can be written as

\[ \psi_j(x) = A_j e^{ik(x-x_j)} + B_j e^{-ik(x-x_j)} \]

in the well and

\[ \phi_j(x) = C_j e^{-\kappa(x-y_j)} + D_j e^{\kappa(x-y_j)} \]

in the barrier. Here,

\[ k = \sqrt{\frac{2m^*_w E}{\hbar^2}}, \quad \kappa = \sqrt{\frac{2m^*_b (V-E)}{\hbar^2}} \]

are the wave numbers in the wells and barriers, respectively.

By applying the Bastard’s matching conditions of the wave function and its derivative at discontinuity of \( V(x) \), we can write the relation of the coefficients between the \( j \)th and \( (j+1) \)th wells as

\[ \begin{pmatrix} A_{j+1} \\ B_{j+1} \end{pmatrix} = T_j \begin{pmatrix} A_j \\ B_j \end{pmatrix} = \begin{pmatrix} \alpha_j & \beta_j \\ \beta_j^* & \alpha_j^* \end{pmatrix} \begin{pmatrix} A_j \\ B_j \end{pmatrix}, \]

where \( T_j \) is the unimodular transfer matrix, and \( \alpha_j \) and \( \beta_j \) are given by

\[ \alpha_j = \left[ \cosh(kb_j) + \frac{i}{2} \left( \frac{m^*_w k}{m^*_b \kappa} - \frac{m^*_b \kappa}{m^*_w k} \right) \sinh(kb_j) \right] e^{ikw_j}, \]

\[ \beta_j = -\frac{i}{2} \left( \frac{m^*_w k}{m^*_b \kappa} + \frac{m^*_b \kappa}{m^*_w k} \right) \sinh(kb_j) e^{-ikw_j}. \]

Here, \( w_j(=y_j-x_j) \) and \( b_j(=x_{j+1}-y_j) \) are the widths of the \( j \)th well and barrier. Multiplying \( T_j \) successively, we can write the relation of \( A \)’s and \( B \)’s between the first and the \((N+1)\)th region as

\[ \begin{pmatrix} A_{N+1} \\ B_{N+1} \end{pmatrix} = M_N \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}, \]

where \( M_N \) is the total transfer matrix given by

\[ M_N = T_N T_{N-1} \cdots T_2 T_1 = \begin{pmatrix} a_N b_N \\ b^*_N a^*_N \end{pmatrix}. \]

Since there will be a reflected wave in the first region but only a transmitted wave in the \((N+1)\)th region (i.e., \( B_{N+1} = 0 \)), we can write the transmission coefficient as

\[ T = \frac{1}{|a_N|^2}. \]

Generally, it requires extensive matrix manipulation to calculate \( T \). However, for the multibarrier systems considered in this paper, \( T \) can be easily calculated in terms of the deterministic substitution rules given below.

We now introduce four kinds of deterministic sequences – the BP, the TM [16,17], the period-doubling (PD) [18], and the copper-mean (CM) [19] sequences which are gen-
erated by the substitution rules

\[ \begin{align*}
BP : S_{l+1} &= S_l^2, \quad S_1 = AB \\
TM : S_{l+1} &= S_l \overline{S_l}, \quad (S_0, S_0) = (B, A) \\
PD : S_{l+1} &= S_l S_{l-1}^2, \quad (S_1, S_1) = (A, AB) \\
CM : S_{l+1} &= S_l S_{l-1}^2, \quad (S_{-1}, S_0) = (B, A),
\end{align*} \]

where \( l \) is the generation number (i.e., \( N = 2^l \) for the first three sequences and \( N = [2^{l+2} - (-1)^l] / 3 \) for the last sequence) and \( \overline{S_l} \) is the complement of \( S_l \) which is obtained by exchanging the letters \( A \) and \( B \). Here, \( A \) and \( B \) represent two kinds of unit cells of the multibarrier system. The unit cell \( A \) (\( B \)) consists of a well with the width \( w_A \) (\( w_B \)) and a barrier with the width \( b_A \) (\( b_B \)) and the height \( V \). We refer the case of \( w_A = w_B \) with \( b_A \neq b_B \) as the CW model and the case of \( b_A = b_B \) with \( w_A \neq w_B \) as the CB model, respectively.

By means of Eq. (11), we can write the recursion relations of the total transfer matrices between different generations as

\[ \begin{align*}
BP : M_{l+1} &= M_l^2, \quad M_1 = T_B T_A \\
TM : M_{l+1} &= \overline{M_l} M_l, \quad (\overline{M_0}, M_0) = (T_B, T_A) \\
PD : M_{l+1} &= M_{l-1} M_l, \quad (M_0, M_1) = (T_A, T_B T_A) \\
CM : M_{l+1} &= M_{l-1} M_l, \quad (M_{-1}, M_0) = (T_B, T_A).
\end{align*} \]

Using the relations in Eq. (12), we can easily derive the recursion relations of \( a \)'s and \( b \)'s between different generations as follows:

\[ \begin{align*}
a_{l+1} &= a_l^2 + b_l b_l \\
b_{l+1} &= b_l(a_l + a_l^*)
\end{align*} \]

with \( a_1 = \alpha_A \alpha_B + \beta_A^* \beta_B \) and \( b_1 = \alpha_B \beta_A + \alpha_A^* \beta_B \) for the BP sequence,

\[ \begin{align*}
a_{l+1} &= \overline{a_l} a_l + b_l \overline{b_l}, \quad b_{l+1} = \overline{a_l} b_l + a_l \overline{b_l} \\
\overline{a_{l+1}} &= a_l \overline{a_l} + b_l \overline{b_l}, \quad \overline{b_{l+1}} = a_l \overline{b_l} + \overline{a_l} \overline{b_l}
\end{align*} \]

with \( a_0 = \alpha_A, \ b_0 = \beta_A, \overline{a_0} = \alpha_B, \) and \( \overline{b_0} = \beta_B \) for the TM sequence, and

\[ \begin{align*}
a_{l+1} &= a_l(a_{l-1}^2 + |b_{l-1}|^2) + b_l^* b_{l-1} (a_{l-1} + a_{l-1}^*) \\
b_{l+1} &= b_l(a_{l-1}^2 + |b_{l-1}|^2) + a_l^* b_{l-1} (a_{l-1} + a_{l-1}^*)
\end{align*} \]

with \( a_0 = \alpha_A, \ b_0 = \beta_A, \ a_1 = \alpha_A \alpha_B + \beta_A^* \beta_B, \) and \( b_1 = \alpha_B \beta_A + \alpha_A^* \beta_B \) for the PD sequence. Recursion relations for the CM sequence are exactly the same as Eq. (15) with \( a_{-1} = \alpha_B, \ b_{-1} = \beta_B, \ a_0 = \alpha_A, \) and \( b_0 = \beta_A \).

3 Numerical results and discussion

As a sample material for calculation, we choose the \( \mu c \)-Si:H/\( a \)-Si:H superlattice [22], where \( \mu c \)-Si:H acts as the well and \( a \)-Si:H the barrier with \( V = 0.4 \) eV. The effective mass in the wells and barriers is taken to be \( m_w^* = m_b^* = 0.3 m_e \) [23], where \( m_e \) is the free electron mass. In calculating transmission coefficients of an electron through multibarrier systems, we treat two cases separately: the one is to set the widths of the wells equal while arrange the widths of the barriers according to the given substitution rule (the CW model), and the other is to set the widths of the barriers equal while arrange the widths of the wells according to the given substitution rule (the CB model). Some examples of the results are plotted in Figures 2 and 3. In plotting, the mesh of \( E \) is taken to be \( \Delta E = 1.0 \times 10^{-5} \) eV, and the system parameters are set
to be $w_A = w_B = 20 \, \text{Å}$ and $b_A = 2b_B = 8 \, \text{Å}$ in the CW model, and $b_A = b_B = 7 \, \text{Å}$ and $w_A = 2w_B = 40 \, \text{Å}$ in the CB model, respectively. Figure 2 shows the results obtained from the CW model for the energy range near the lowest domain of resonances, and Figure 3 shows the results obtained from the CB model for the energy range near the first two lowest domains of resonances. Here, the ‘domain of resonances’ means the energy range that contains resonant peaks in the finite-size system and would approach the allowed energy band in the infinite limit of the system size.

We first discuss the features of the transmission resonances exhibited in the BP system with $l = 2$. In this case, three resonant peaks in each domain of resonances are expected due to overlap of quasi-bound states in the three well regions, and the result obtained from the CW model [Figure 2a] agrees well with the expectation. An interesting feature to be noted in Figure 2a is that the first and the third peaks of the three resonant peaks are complete (i.e., $T = 1$) while the second peak is incomplete (i.e., $T < 1$). We will see that the two complete peaks locate in the middle of the subdomains while the incomplete peak disappears for large $l$ [see Figure 2e]. As for the result obtained from the CB model [Figure 3a], there are two distinctive features from the result obtained from the CW model. The one is that there occurs suppression of resonant peaks. We can see in Figure 3a that there exist a single complete peak in the first lowest domain and two complete peaks in the second lowest domain, which implies that two peaks in the first lowest domain and one peak in the second lowest domain are suppressed. The second is that the resonance widths exhibited in the CB model are much narrower and sharper than those in the CW model.

We now discuss the features of the transmission resonances in the BP system with large $l$. As $l$ increases, successive resonant splitting effects and the energy band effects on the transmission properties are expected, and we confirm them. Figure 2e shows the transmission coefficients obtained from the CW model with $l = 5$. Here two distinctive features from the case of the periodic system [12-14] are emerged. The first is that the main domain splits into two subdomains, the centers of which correspond to the first and the third resonant peaks in Fig-
different behavior; no splitting into subdomains occurs, which indicates that the binary periodicity of the system does not affect on the splitting of this domain.

We also study the features of the transmission resonances with varying the widths of the wells and barriers, and observe that the number of resonance domains increases with increasing the width of the well, which can be easily understood by noting that the energies of the quasi-bound states in a well are approximately in proportional to the inverse square of the width of the well [24]. We also observe that the widths of resonance domains decrease and the peak-to-valley ratios increase with increasing the width of the barrier.

Having seen the features of the transmission resonances in the BP system, we now discuss the features of the transmission resonances exhibited in the aperiodic TM, PD, CM systems with \( l = 2 \). In this case, the three, three, and four resonant peaks are expected to exist in each domain of resonances due to overlap of quasi-bound states in the three, three, and four wells of the TM, PD, CM systems. The results obtained from the CW model for these systems are plotted in Figures 2b – 2d, where it can be seen that the number of resonant peaks fits with the expectation. However, the results obtained from the CB model [Figures 3b – 3d] do not always fit with the expectation: The transmission coefficients for the second lowest domain agree with the expectation, while the number of resonant peaks in the first lowest domain is less than the expected number due to suppression of the peaks. The number of suppressed peaks is two, one, and one in the TM, PD, CM systems.
system, respectively. As for the effects of aperiodicity, we would like to mention two points. The first is that the lowest resonant peaks shift towards the lower energy region, compared with that of the BP system. The second is that there coexist the complete and incomplete resonant peaks. For the peaks exhibited in the CW model, all the peaks in the TM system and the second peak in the CM system are complete, while all the peaks in the PD system and all the peaks expect the second peak in the CM system are incomplete. In the meanwhile, for the peaks exhibited in the CB model, all the peaks are incomplete, which implies that it is more difficult for an electron to tunnel through the CB structure than the CW structure. Here it should be noted that the incomplete resonant peak appeared in the BP system [Figure 2a] and the incomplete peaks appeared in the aperiodic systems show different behavior as $l$ increases; the former fails to locate in the middle of the subbands and disappears, while the latter survives to locate in the middle of the subdomains.

4 Summary

In summary, we studied the effects of aperiodicity on the transmission resonances of an electron through a few types of binary aperiodic multibarrier systems with finite system size. Dependence of transmission resonances on the system parameters was investigated, from which the similarities and differences of the resonances between the binary periodic and aperiodic systems were presented. In doing this, a comparison of resonance splitting exhibited in the common-well structure with those exhibited in the common-barrier structure of the multibarrier systems was also made in detail. It was found that complex resonance
splitting and a variety of peak-to-valley ratios which are not exhibited in the periodic system are emerged as a result of introducing aperiodicity. It was also found that the transmission resonances for some energy ranges in the aperiodic systems resemble those in the periodic system, despite the existence of aperiodicity. We hope that exotic resonant tunneling properties of the binary aperiodic multibarrier systems such as the complex resonance splitting effects, deep levels of hierarchy in the peak-to-valley ratios, and the existence of tunneling plateaus can be applied in designing a new type of electronic device.

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