PHYSICAL REVIEW B VOLUME 44, NUMBER 11 15 SEPTEMBER 1991-I

General formalism of the Kronig-Penney model suitable for superlattice applications

Shao-hua Pan
*China Center of Advanced Science and Technology (World Laboratory), P.O. Box 8730, Beijing 100 080, China and Institute of Physics, Academia Sinica, P.O. Box 603, Beijing 100 080, China**

Si-min Feng
Institute of Physics, Academia Sinica, P.O. Box 603, Beijing 100 080, China
(Received 30 July 1990)

A formalism of the Kronig-Penney model has been developed that is more general than that of Cho and Prucnal [Phys. Rev. B **36**, 3237 (1987)]. It gives not only odd- and even-index subbands but also wave functions for all values of the wave number. A parity analysis of the wave functions is also given.

I. INTRODUCTION

Superlattices (SL's) and multiple-quantum-well structures (MQWS's) are alternating ultrathin epitaxial layers with different constituent-semiconductor compositions, e.g., GaAs and $Al_xGa_{1-x}As$. Because of the band offset of the heterolayers, smaller energy gap layers act as potential wells between larger energy gap layers. Figure 1 shows the periodic square potential of a superlattice with well width a, barrier width b, and barrier height V. Since the superlattice period $d=a+b$ is much longer than the original lattice constant of the host crystal, the Brillouin zone is divided into a series of minizones, giving rise to narrow subbands separated by forbidden regions. As a consequence, the actual wave function of a superlattice can be separated into a product of a Bloch wave function with a period equal to the atomic lattice constant, and an envelope wave function of the superlattice potential.

Cho and Prucnal[1] calculated the envelope wave functions at the edges of each subband (corresponding to the superlattice wave number $k=0$ and π/d). These envelope wave functions are useful to analyze the superlattice properties. The purpose of this paper is to give the envelope wave functions for all values of k, and to show that the wave functions corresponding to the values of k other than zero or π/d have mixed parities in general.

II. ODD- AND EVEN-INDEX ENERGY BANDS

From the solution of the Schrödinger equation the envelope wave function in the period $-b\le z\le a$ can be written as

$$\psi(z)=\begin{cases}\psi_{0+}\cos(\alpha z)+\dfrac{1}{\alpha}\psi'_{0+}\sin(\alpha z)\ , & 0\le z\le a\\[2ex] \psi_{0-}\cosh(\delta z)+\dfrac{1}{\delta}\psi'_{0-}\sinh(\delta z)\ , & -b\le z\le 0\ .\end{cases} \tag{1}$$

Here $\psi_{0\pm}$ and $\psi'_{0\pm}$ denote $\psi(z)|_{z=\pm 0}$ and $d\psi(z)/dz|_{z=\pm 0}$, respectively, α and δ are defined as

$$\alpha\equiv(2m_aE)^{1/2}/\hbar\ ,\qquad \delta\equiv[2m_b(V-E)]^{1/2}/\hbar\ , \tag{2}$$

where E is the electron energy, and m_a and m_b are the effective masses at the well and at the barrier, respectively. The inverse $1/\delta$ of δ is called the wave-function penetration depth in the barrier. For simplicity we consider the case of $E<V$ only; the extension to the case of $E>V$ is straightforward. The wave function $\psi(z)$ in other periods can be obtained by using Bloch's theorem and Eq. (1). Using Bastard's boundary condition[2] at $z=0$, i.e., $\psi_{0+}=\psi_{0-}\equiv\psi_0$ and $\psi'_{0+}/m_a=\psi'_{0-}/m_b$, and applying the relation $\psi(a)=\psi^-(-b)\exp(ikd)$ from Bloch's theorem, we can eliminate ψ'_{0+} and ψ'_{0-} from Eq. (1) to obtain

$$\psi(z)=\begin{cases}\psi_0[\cos(\alpha z)+\gamma P\sin(\alpha z)], & 0\le z\le a\\ \psi_0[\cosh(\delta z)+P\sinh(\delta z)], & -b\le z\le 0\ ,\end{cases} \tag{3}$$

where γ and P are defined as

$$\gamma\equiv\delta m_a/\alpha m_b\ , \tag{4}$$

$$P\equiv\frac{\cosh(\delta b)\exp(ikd)-\cos(\alpha a)}{\gamma\sin(\alpha a)+\sinh(\delta b)\exp(ikd)}\ . \tag{5}$$

From Eqs. (3) and (5) we can directly verify the symmetry relations in the periodic square potential

$$|\psi(a/2+x)|=|\psi(a/2-x)|,\quad |x|\le a/2\ ; \tag{6a}$$

and

$$|\psi(-b/2+x)|=|\psi(-b/2-x)|,\quad |x|\le b/2\ . \tag{6b}$$

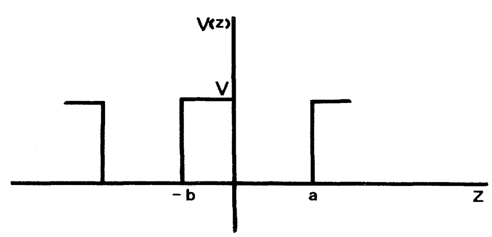

FIG. 1. The periodic square potential of a superlattice; a is the well width, b is the barrier width, V is the barrier height.

Substituting Eqs. (3) and (5) into the normalization condition

$$\int_{-b}^{a} |\psi(z)|^2 dz = 1$$

and using the symmetry relations (6a) and (6b) to simplify the result, we obtain

$$\psi_0 = \left[a \left[\frac{1+\gamma^2|P|^2}{2} + \frac{\gamma\,\mathrm{Re}(P)}{\alpha a} \right] + b \left[\frac{1-|P|^2}{2} + \frac{\mathrm{Re}(P)}{\delta b} \right] \right]^{-1/2} , \tag{7}$$

where Re(P) denotes the real part of P.

Using Bloch's theorem and Bastard's boundary condition we have

$$\psi'(a-0) = \psi'(-b-0)\exp(ikd) = (m_a/m_b)\psi'(-b+0)\exp(ikd) .$$

Substituting Eqs. (3) and (5) into this equation we obtain

$$\cos(kd) = \cos(\alpha a)\cosh(\delta b) + \tfrac{1}{2}(\gamma - 1/\gamma)\sin(\alpha a)\sinh(\delta b) , \tag{8}$$

the same equation as that derived in Ref. 1.

Equation (8) is useful in analyzing the connection and distinction between MQWS's and SL's. The distinction between MQWS's and SL's depends on the relative magnitude of the barrier width b and of the wave-function penetration depth in the barrier $1/\delta$.[3] In MQWS's, $b \gg 1/\delta$, i.e., $\delta b \gg 1$, so most of the physical properties are those of a series of uncoupled wells. Conversely, in SL's, $b < 1/\delta$, i.e., $\delta b < 1$, and the tunnel coupling among wells significantly modifies the physical properties of the system. In particular, tunnel coupling results in the broadening of the energy levels into subbands with finite widths. The situation can be seen more clearly by rewriting Eq. (8) as

$$\gamma = \frac{\cos(kd) - \cos(\alpha a)\cosh(\delta b)}{\sin(\alpha a)\sinh(\delta b)} - \frac{(-1)^j\{[\cosh(\delta b) - \cos(kd)\cos(\alpha a)]^2 - \sin^2(kd)\sin^2(\alpha a)\}^{1/2}}{\sin(\alpha a)\sinh(\delta b)} , \tag{9}$$

where the index j indicates the two sets of solutions for γ and j can be any odd or even number. When $\delta b \gg 1$, Eq. (9) can be simplified as

$$\gamma = \begin{cases} \tan(\alpha a/2), & j = 1,3,5,\dots \\ -\cot(\alpha a/2), & j = 2,4,6,\dots . \end{cases} \tag{10}$$

These results correspond, respectively, to odd- and even-index energy levels in a single well.[4] When δb becomes smaller the terms with k in Eq. (9) cannot be neglected, resulting in a band structure with finite width. Since the index j in Eq. (10) indicates the order of the energy levels, and since the $\pm$ signs, i.e., $-(-1)^j$, before the radical expression in Eq. (9) cannot be changed abruptly when δb becomes smaller, we can judge that j in Eq. (9) represents the index of the subband. For example, from Eq. (9), we can obtain

$$\gamma = \begin{cases} \tan(\alpha a/2)\coth(\delta b/2) & \text{for } j = 1,3,5,\dots \text{ and } kd = 0 \\ \tan(\alpha a/2)\mathrm{tnh}(\delta b/2) & \text{for } j = 1,3,5,\dots \text{ and } kd = \pi \\ -\cot(\alpha a/2)\coth(\delta b/2) & \text{for } j = 2,4,6,\dots \text{ and } kd = \pi \\ -\cot(\alpha a/2)\tanh(\delta b/2) & \text{for } j = 2,4,6,\dots \text{ and } kd = 0 . \end{cases} \tag{11}$$

Note that both $kd = 0$ of odd-index bands and $kd = \pi$ of even-index bands correspond to minimum energies; both $kd = \pi$ of odd-index bands and $kd = 0$ of even-index bands correspond to maximum energies. Equation (11) is identical to the edge-energy equations in Ref. 1 which can thus be regarded as special cases of Eq. (9) of this paper.

III. PARITIES OF ENVELOPE WAVE FUNCTIONS

We first consider the case of $\delta b \gg 1$. Substituting Eqs. (5) and (10) into Eq. (3) we obtain the wave function for the barrier $\psi_0\exp(-\delta|z|)$ and the wave functions in the well

$$\psi(z) = \begin{cases} A_0\cos[\alpha(z-a/2)], & j = 1,3,5,\dots \\ B_a\sin(\alpha(z-a/2)], & j = 2,4,6,\dots , \end{cases} \tag{12a}$$

where

$$A_0 = \psi_0/\cos(\alpha a/2), \quad B_0 = -\psi_0/\sin(\alpha a/2) . \tag{12b}$$

The wave functions in Eq. (12a) have even parity for $j=1,3,5,\ldots$ and odd parity for $j=2,4,6,\ldots,$. These are identical to the well-known results for a single well. When δb becomes smaller the wave functions have the following more general forms:

$$\psi(z)=\begin{cases} A\cos[\alpha(z-a/2)]+B\sin[\alpha(z-a/2)], & 0\le z\le a \\ C\cosh[\delta(z+b/2)]+D\sinh[\delta(z+b/2)], & -b\le z\le 0\ . \end{cases} \tag{13}$$

By comparing the two sets of expressions for $\psi(z)$, Eqs. (3) and (13), we obtain the new coefficients

$$A=\psi_0[\cos(\alpha a/2)+\gamma P\sin(\alpha a/2)]\ , \tag{14a}$$

$$B=\psi_0[\gamma P\cos(\alpha a/2)-\sin(\alpha a/2)]\ , \tag{14b}$$

$$C=\psi_0[\cosh(\delta b/2)-P\sinh(\delta b/2)]\ , \tag{14c}$$

$$D=\psi_0[P\cosh(\delta b/2)-\sinh(\delta b/2)]\ . \tag{14d}$$

Substituting Eqs. (5) and (11) into Eq. (3), or equivalently, substituting Eqs. (5), (11), and (14) into Eq. (13), we obtain for $j=1,3,5,\ldots$ and $kd=0$,

$$\psi(z)=\begin{cases} A_0\cos[\alpha(z-a/2)], & 0\le z\le a \\ C_0\cosh[\delta(z+b/2), & -b\le z\le 0\ ; \end{cases} \tag{15a}$$

for $j=1,3,5,\ldots$ and $kd=\pi$,

$$\psi(z)=\begin{cases} A_0\cos[\alpha(z-a/2)], & 0\le z\le a \\ D_0\sinh[\delta(z+b/2)], & -b\le z\le 0\ ; \end{cases} \tag{15b}$$

for $j=2,4,6,\ldots$ and $kd=\pi$,

$$\psi(z)=\begin{cases} B_0\sin[\alpha(z-a/2)], & 0\le z\le a \\ C_0\cosh[\delta(z+b/2)], & -b\le z\le 0\ ; \end{cases} \tag{15c}$$

and for $j=2,4,6,\ldots$ and $kd=0$,

$$\psi(z)=\begin{cases} B_0\sin[\alpha(z-a/2)], & 0\le z\le a \\ D_0\sinh[\delta(z+b/2)], & -b\le z\le 0 \end{cases} \tag{15d}$$

where $C_0=\psi_0/\cosh(\delta b/2)$, $D_0=\psi_0/\sinh(\delta b/2)$. Equations (15a)–(15d) are identical to the equations of wave function at the edges for odd- and even-index bands in Ref. 1 which were obtained by the observation that the wave functions corresponding to maximum and minimum energies of each band have definite parities. The equations of Ref. 1 can thus be regarded as special cases of Eq. (13) of this paper.

Although the wave functions at the edges of each band have definite parities, Eq. (13) shows that the wave functions corresponding to values of kd other than zero and π have mixed parities in general. To see this fact more clearly we rewrite Eq. (14) as

$$A=\begin{cases} A_0[1-(R+iI), & j=1,3,5,\ldots \\ A_0(R+iI), & j=2,4,6,\ldots, \end{cases} \tag{16a}$$

$$B=\begin{cases} B_0(R+iI), & j=1,3,5,\ldots \\ B_0[1-(R+iI)], & j=2,4,6,\ldots, \end{cases} \tag{16b}$$

and similar expressions of C and D, where

$$I=(-1)^j\frac{\gamma}{2}\frac{\sin(kd)\sin(\alpha a)[\gamma\sin(\alpha a)\cosh(\delta b)+\cos(\alpha a)\sinh(\delta b)]}{[\cos(kd)\sinh(\delta b)+\gamma\sin(\alpha a)]^2+[\sin(kd)\sinh(\delta b)]^2}\ , \tag{17}$$

$$R=\tfrac{1}{2}[1-(1-4I^2)^{1/2}]\ . \tag{18}$$

In obtaining Eq. (18) we have applied Eq. (6a) to simplify the result. $|R|$ is a monotonic increasing function of $|I|$ and $R=0$ when $I=0$. According to Eqs. (12a) and (16), we can define the parity-mixing degree $M_p(k)$ as follows:

$$M_p(k)=\left[\frac{R^2+I^2}{(1-R)^2+I^2}\right]^{1/2}\ . \tag{19}$$

We denote the maximum of $M_p(k)$ by $\max\{(M_p)_j\}$ with a subband-index j as the subscript. Since α, δ, and γ are also functions of k, Eqs. (17)–(19) indicate that $M_p(k)$ is a complicated function of k. Obviously, $M_p(k)=0$ when $kd=0$ and $\pm\pi$, i.e., at the band edges. The $\max\{(M_p)_j\}$, in general, occurs at a k value far from the band edges. As a first example, for a $GaAs/Al_{a3}Ga_{0.7}As$ superlattice with well width $a=90$ Å, and barrier width $b=120$ Å, $\max\{(M_p)_1\}=0.035\%$ (corresponding to $\delta b=8.5$), and $\max\{(M_p)_2\}=0.18\%$ ($\delta b=6.0$). These both occur at the centers of the subbands, i.e., $kd=\pm\pi/2$. As another example, for the same kind of superlattice with the same well width but a different barrier width, $b=5$ Å, $\max\{(M_p)_1\}=97\%$ ($\delta b=0.36$) at $kd=\pm 0.57\pi$, and $\max\{(M_p)_2\}=99\%$ ($\delta b=0.20$) at $kd=\pm 0.37\pi$.

The tunnel coupling among quantum wells results in the mixing of energy levels with different parities. When the tunnel coupling is negligible, i.e., when $\delta b\gg 1$, Eq. (17) shows that I, and hence R and $M_p(k)$ approach zero, as they should. Conversely, when the tunnel coupling is strong, i.e., when $\delta b<1$, the mixing of heteroparities is obvious. Thus, when the well width a and barrier height V (which is determined by the composition percentage x) are given, e.g., for $GaAs/Al_xGa_{1-x}As$ superlattices, the mixing of heteroparities becomes more obvious when the barrier width b becomes smaller. This conclusion is also

TABLE I. The maximum parity-mixing degrees $\max\{(M_p)_j\}$ for the first and second subbands in $GaAs/Al_{0.25}Ga_{0.75}As$ superlattices with well width $a = 100$ Å, and different barrier widths b.

b (Å)	150	130	110	90	70	50	30	10
$\max\{(M_p)_1\}$ (%)	0.014	0.048	0.17	0.59	2.1	7.2	26	98
$\max\{(M_p)_2\}$ (%)	0.092	0.23	0.55	1.3	3.3	8.2	22	95

confirmed by the two examples given. In order to see this trend more clearly we summarize a set of calculated results in Table I. As is well known, the tunnel broadening subband width ΔE_j is always greater for larger j (higher subbands), but this does not mean that $(M_p)_j$ is also always greater for larger j, as shown in Table I. This is due to the fact that the parity mixing comes from the interaction, i.e., the mutual influence (penetration) between higher and lower subbands.

IV. CONCLUSION

Using Bloch's theorem and Bastard's boundary condition followed by analysis of the connection and distinction between the weak tunnel coupling case, $\delta b \gg 1$, and the strong tunnel coupling case, $\delta b < 1$, we have derived the odd- and even-index energy subbands and the wave functions corresponding to all values of k. The eigenenergies and wave functions at the edges of each band in Ref. 1 can be regarded as special cases in this paper.

As pointed out by the authors of Ref. 1, the new formalism in Ref. 1, in particular, its expressions for the wave functions corresponding to the edge energies of each band, is very useful for the analysis of superlattices and applications to device designs. According to our numerical calculations, for usual doping concentrations of about $10^{18}/cm^3$, the Fermi level at room temperature is often above the maximum energies of the first (ground) subband in superlattices, hence the wave functions corresponding to all values of k are necessary for detailed analysis of intersubband optical transitions between the first (ground) subband and the next excited subbands. We thus believe that the new formalism in this paper is a more general one which is more suitable for the analysis and applications of superlattices.

The tunnel coupling among wells results in the mixing of energy levels of different parities. The wave functions corresponding to values of k other than zero and π/d have mixed parities in general. These superlattice properties give rise to greater details in the interband and intersubband optical transition processes because the optical transition selection rules are related to the parities of wave functions. It may be possible in the future to apply this new general formalism to analyze nonlinear optics phenomena in superlattices.

Although this formalism has been derived to be suitable for superlattice applications it is also applicable to bulk materials by letting $m_a = m_b$.

*Mailing address.

[1]H.-S. Cho and P. R. Prucnal, Phys. Rev. B **36**, 3237 (1987).
[2]G. Bastard, Phys. Rev. B **24**, 5693 (1981).
[3]D. S. Chemla and D. A. B. Miller, J. Opt. Soc. Am. B **2**, 1155 (1985).
[4]H. Kawai, K. Kaneko, and N. Watanabe, J. Appl. Phys. **56**, 463 (1984).