New formalism of the Kronig-Penney model with application to superlattices

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A new formalism of the Kronig-Penney model has been developed which is considerably simpler than the conventional one. It gives not only the carrier energy bands but also the wave functions at the edges of each band. Although it is formulated to be applied to superlattices, it is also applicable to bulk materials.

I. INTRODUCTION

The Kronig-Penney model[1] is an idealized method of calculating the energy bands in crystalline solids with periodically varying potentials. It has been applied primarily to bulk semiconductors[2,3] to study the qualitative nature of band structures. Recently, it has also been applied to semiconductor superlattices[4–7] to calculate quantum confined energy subbands. Here, because of conduction- and valence-band discontinuities, smaller–energy-gap layers act as potential wells between larger–energy-gap layers. Though the effective mass of carriers is the same throughout bulk materials, it is different in the well and barrier layers of superlattice structures. This effective mass difference must be taken into account by the appropriate boundary condition at the well/barrier interface. The conventional formalism of the Kronig-Penney model for bulk materials must therefore be modified for superlattices.

Mukherji and Nag[4] considered the effective-mass difference in formulating the Kronig-Penney model, but assumed that the wave function and its first derivative were continuous at the interface. Bastard[5] replaced the assumption of continuity of the first derivative of wave function with an envelope function approximation. He showed that the first derivative of the wave function divided by effective mass, or the probability current, is continuous at the interface under certain conditions. Although several other boundary conditions have been proposed,[8–10] Bastard's is the simplest and most intuitively appealing. The results of particle energy calculations based on Bastard's boundary condition are consistent with the experimental data.[11] Recently, the Kronig-Penney model with Bastard's boundary condition was also used to calculate the band offset of GaAs/Al_xGa_{1-x}As superlattices.[12]

The purpose of this paper is to present a new formalism of the Kronig-Penney model developed using Bastard's boundary condition. This formalism is based on the observation that wave functions corresponding to maximum and minimum energies of each band have definite parities. Since this formalism is simpler and easier to manipulate than the conventional formalism, it can be used to find energy bands and wave functions in superlattices and bulk materials by simple numerical analysis. In the following section, both the conventional formalism, and the new formalism of the Kronig-Penney model with Bastard's boundary condition, will be developed and compared. In Sec. III application of the new formalism will be illustrated by finding the energy subbands and envelope wave functions of a GaAs/Al_xGa_{1-x}As superlattice. This application will then be discussed.

II. FORMULATION

The periodic potential in a superlattice is not a real atomic potential, but a periodic repetition of different energy gap layers, the thickness of which is usually many times larger than the period of the atomic potential. As a consequence, the actual wave function of a superlattice is a bulk atomic wave function modulated by the envelope wave function of the superlattice potential. The energy bands of a superlattice are composed of a discrete series of subbands induced by the superlattice potential inside a bulk band.

In this section, we will formulate the energy subbands and envelope wave functions induced by the superlattice potential, using a new formalism of the Kronig-Penney model and applying Bastard's boundary condition. Before developing the new formalism, the conventional formalism is first developed for comparison.

A. Conventional formalism

Figure 1 shows the periodic square potential of a superlattice with well thickness a, barrier thickness b, and barrier height V. Particle effective mass is m_a at the well and m_b at the barrier. From the solution of the Schrödinger equation, the envelope wave function in two adjacent periods, $-b<z<a$ and $a<z<d+a$, can be written as

$$\Psi(z)=\begin{cases} Ae^{i\alpha(z-a/2)}+Be^{-i\alpha(z-a/2)}\equiv\Psi_a(z), & 0\leq z\leq a \\ Ce^{i\beta(z+b/2)}+De^{-i\beta(z+b/2)}\equiv\Psi_b(z), & -b\leq z\leq 0 \end{cases}, \tag{1}$$

$$\Psi(z)=\begin{cases} e^{i\Phi}[Ae^{i\alpha(z-a/2-d)}+Be^{-i\alpha(z-a/2-d)}]\equiv\Psi_c(z), & d\leq z\leq d+a \\ e^{i\Phi}[Ce^{i\beta(z+b/2-d)}+De^{-i\beta(z+b/2-d)}]\equiv\Psi_d(z), & a\leq z\leq d \end{cases}, \tag{2}$$

where $d=a+b$ is the period of the superlattice, A, B, C, and D are complex numbers, $e^{i\Phi}$ is the phase factor, and z is the axis perpendicular to the superlattice layers. α and β are defined as

$$\alpha \equiv \frac{1}{\hbar}(2m_a E)^{1/2} ,$$

$$\beta \equiv \frac{1}{\hbar}[2m_b(E-V)]^{1/2} ,$$

where E is the particle energy. Ψ_a, Ψ_b, Ψ_c, and Ψ_d are defined only inside a well or a barrier. We note $|\Psi_a(0)| = |\Psi_a(a)|$ and $|\Psi_b(-b)| = |\Psi_b(0)|$ from the symmetry of the wells and barriers, and also note $|\Psi(z+d)| = |\Psi(z)|$ from the periodicity of superlattice potential. Using Bastard's boundary condition at $z=0$ and $z=a$, i.e.,

$$\Psi_a(0)=\Psi_b(0), \quad \frac{1}{m_a}[\Psi_a'(z)]_{z=0}=\frac{1}{m_b}[\Psi_b'(z)]_{z=0} ,$$

$$\Psi_a(a)=\psi_d(a), \quad \frac{1}{m_a}[\Psi_a'(z)]_{z=a}=\frac{1}{m_b}[\Psi_d'(z)]_{z=a} ,$$

where $\Psi_a'(z)$ and $\Psi_b'(z)$ are the first derivatives of $\Psi_a(z)$ and $\Psi_b(z)$, respectively, and applying the condition that A, B, C, and D should not be zero simultaneously, we obtain

$$\begin{vmatrix} 1 & 1 & 1 & 1 \\ \frac{\alpha}{m_a} & -\frac{\alpha}{m_a} & \frac{\beta}{m_a} & -\frac{\beta}{m_a} \\ e^{i\alpha a} & e^{-i\alpha a} & e^{i(\Phi-b\beta)} & e^{i(\Phi+b\beta)} \\ \frac{\alpha}{m_a}e^{i\alpha a} & -\frac{\alpha}{m_a}e^{-i\alpha a} & \frac{\beta}{m_b}e^{i(\Phi-b\beta)} & -\frac{\beta}{m_b}e^{i(\Phi+b\beta)} \end{vmatrix} = 0 .$$

Note that by Bloch's theorem $\Psi(z)=e^{ikz}u(z)$, where k is the wave number of the envelope function in the z axis and $u(z)$ is a periodic potential satisfying $u(z)=u(z+d)$. It is obvious that $\Psi(z+d)=e^{ikd}e^{ikz}u(z+d)$ is $e^{ikd}\Psi(z)$. Thus Φ is equal to kd. By simplifying the above determinant and replacing Φ by kd, we obtain

$$\cos(kd)=\cos\left[\frac{a}{\hbar}(2m_aE)^{1/2}\right]\cosh\left[\frac{b}{\hbar}[2m_b(V-E)]^{1/2}\right] + \frac{\left[\frac{m_a}{m_b}\right]^{1/2}V-\left[\left[\frac{m_a}{m_b}\right]^{1/2}+\left[\frac{m_b}{m_a}\right]^{1/2}\right]E}{2\sqrt{E(V-E)}}\sin\left[\frac{a}{\hbar}(2m_aE)^{1/2}\right]\sinh\left[\frac{b}{\hbar}[2m_b(V-E)]^{1/2}\right] \quad \text{for } V>E , \tag{3}$$

and

$$\cos(kd)=\cos\left[\frac{a}{\hbar}(2m_aE)^{1/2}\right]\cos\left[\frac{b}{\hbar}[2m_b(E-V)]^{1/2}\right] + \frac{\left[\frac{m_a}{m_b}\right]^{1/2}V-\left[\left[\frac{m_a}{m_b}\right]^{1/2}+\left[\frac{m_b}{m_a}\right]^{1/2}\right]E}{2\sqrt{E(E-V)}}\sin\left[\frac{a}{\hbar}(2m_aE)^{1/2}\right]\sin\left[\frac{b}{\hbar}[2m_b(E-V)]^{1/2}\right] \quad \text{for } V<E , \tag{4}$$

where $\hbar=h/2\pi$ and h is the Planck's constant.

Similar equations have been derived by Bastard,[5] who also included the effect of momentum in the direction parallel to the layers. If continuity of $d\Psi(z)/dz$ is adopted instead of $(1/m)d\Psi(z)/dz$, $(m_a/m_b)^{1/2}$ is replaced by $(m_b/m_a)^{1/2}$ and vice versa, and the overall energy bands shift upward.[11] From Eqs. (3) and (4) the E-k dispersion relations can be readily obtained.

B. New formalism

Even though the conventional formalism yields the energy bands of superlattices or bulk materials, it is quite complicated and cannot yield the envelope wave functions. A new formalism, which will be developed here, is simpler than the conventional formalism, and yields the envelope wave functions corresponding to the edge ener-

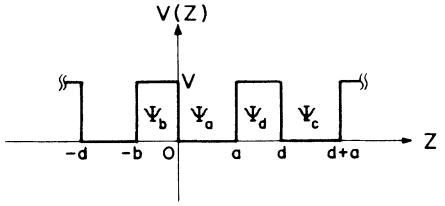

FIG. 1. A schematic view of the periodic square potential of a superlattice. a is the well thickness, b is the barrier thickness, $d=a+b$ is the period of the superlattice, and V is the barrier height. Ψ_a and Ψ_c are the envelope wave functions in the wells at $0<z<a$ and $d<z<d+a$, respectively. Ψ_b and Ψ_d are the envelope wave functions in the barriers at $-b<z<0$ and $a<z<d$, respectively.

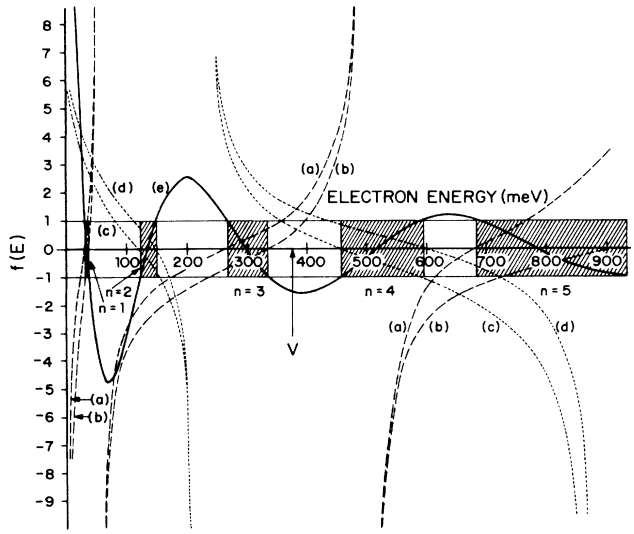

FIG. 2. The first five electron energy subbands of a GaAs/$Al_xGa_{1-x}As$ superlattice with $x=0.5$, $a=100$ Å, and $b=25$ Å. $V=375$ meV is the barrier potential height. Dashed curves (a) and (b) correspond to the functions in the left-hand side of Eqs. (7) and (8), and (11) and (12), respectively. Dotted curves (c) and (d) correspond to the functions in the left-hand side of Eqs. (15) and (16), and (19) and (20), respectively. Solid curve (e) corresponds to the right-hand side of Eqs. (3) and (4), respectively. n is the band index.

gies of each band. These envelope wave functions are useful to analyze the superlattice properties.

From Eqs. (3) and (4), the phase difference ($\Phi=kd$) between $\Psi(z)$ and $\Psi(z+d)$ is 0 or $\pm\pi$ for the wave function corresponding to minimum and maximum energy of each band. The phase difference between $\Psi_a(0)$ and $\Psi_c(d)$ is the sum of the phase difference Φ_a between $\Psi_a(0)$ and $\Psi_a(a)$, and the phase difference Φ_b between $\Psi_a(a)$ and $\Psi_d(d)$. When A is different from B or $-B$ in Eq. (1), Φ_a is different from 0 or $\pm\pi$. Similarly, when C is different from D or $-D$ in Eq. (1), Φ_b is also different from 0 or $\pm\pi$. In general, when Φ_a and Φ_b do not have even or odd parity (when $A\neq B$ or $-B$, or $C\neq D$ or $-D$), the total phase difference cannot be 0 or $\pm\pi$. Therefore, the envelope wave functions corresponding to the minimum and maximum energy of each band must have even or odd parity.

1. *Odd-index bands ($n=1,3,5,\ldots$)*

As will be shown in Fig. 2, the minimum energy of every odd-index band corresponds to $\cos\Phi=1$ or $\Phi=0$. Following the above arguments, Φ_a and Φ_b should both be even or both be odd at minimum energies. Note, however, that at large b each band in a well degenerates to an energy level with vanishing bandwidth. Thus $\Psi_a^{\min}$ (corresponding to minimum energy) and $\Psi_a^{\max}$ (corresponding to maximum energy) become identical. Hence, the parities of $\Psi_a^{\min}$ and $\Psi_a^{\max}$ must be the same for any value of b. Furthermore, Ψ_a is even for the first (ground) state, odd for the second state, and alternating even and odd with increasing n. Therefore, both $\Psi_a^{\min}$ and $\Psi_b^{\min}$ of every odd-index band have even parity, and can be written as

$$\Psi_a^{\min}(z)=A\cos\left[\alpha\left[z-\frac{a}{2}\right]\right],\quad \Psi_b^{\min}(z)=B\cosh\left[\delta\left[z+\frac{b}{2}\right]\right]\quad \text{for } V>E\ , \tag{5}$$

$$\Psi_a^{\min}(z)=A\cos\left[\alpha\left[z-\frac{a}{2}\right]\right],\quad \Psi_b^{\min}(z)=B\cos\left[\beta\left[z+\frac{b}{2}\right]\right]\quad \text{for } V<E\ , \tag{6}$$

where $\delta=i\beta=[2m_b(V-E)]^{1/2}/\hbar$.

Using Bastard's boundary condition at $z=0$, i.e.,

$$\Psi_a(0)=\Psi_b(0)$$

and

$$\frac{1}{m_a}[\Psi_a'(z)]_{z=0}=\frac{1}{m_b}[\Psi_b'(z)]_{z=0}\ ,$$

we obtain

$$A\cos\left[\frac{a\alpha}{2}\right]=B\cosh\left[\frac{b\delta}{2}\right],\quad \frac{A}{m_a}\alpha\sin\left[\frac{a\alpha}{2}\right]=\frac{B}{m_b}\delta\sinh\left[\frac{b\delta}{2}\right]\quad \text{for } V>E\ ,$$

$$A\cosh\left[\frac{a\alpha}{2}\right]=B\cos\left[\frac{b\delta}{2}\right],\quad \frac{A}{m_a}\alpha\sin\left[\frac{a\alpha}{2}\right]=\frac{-B}{m_b}\beta\sin\left[\frac{b\beta}{2}\right]\quad \text{for } V<E\ ,$$

which in turn gives the minimum energy of every odd-index band:

$$\tan\left[\frac{a}{2\hbar}(2m_aE_{\min})^{1/2}\right]-\left[\frac{m_a}{m_b}\left[\frac{V}{E_{\min}}-1\right]\right]^{1/2}\tanh\left[\frac{b}{2\hbar}[2m_b(V-E_{\min})]^{1/2}\right]=0\quad \text{for } V>E\ , \tag{7}$$

$$\tan\left[\frac{a}{2\hbar}(2m_aE_{\min})^{1/2}\right]+\left[\frac{m_a}{m_b}\left[1-\frac{V}{E_{\min}}\right]\right]^{1/2}\tan\left[\frac{b}{2\hbar}[2m_b(E_{\min}-V)]^{1/2}\right]=0\quad \text{for } V<E\ . \tag{8}$$

The smallest solution of Eq. (7) corresponds to $n=1$ (ground subband), the next solution to $n=3$, etc. The band index corresponding to the smallest solution of Eq. (8) depends on how many bands are confined inside the well.

To find the maximum energy of each odd-index band, we note that $\cos\Phi$ is -1 or Φ is $\pm\pi$. Φ_a is 0 because Ψ_a is even. Since $\Phi_a+\Phi_b$ is $\pm\pi$, Φ_b is $\pm\pi$, or Φ_b is odd. Hence, the wave functions can be written as

$$\Psi_a^{\max}(z)=A\cos\left[\alpha\left[z-\frac{a}{2}\right]\right],\quad \Psi_b^{\max}=B\sinh\left[\delta\left[z+\frac{b}{2}\right]\right]\quad \text{for } V>E\ , \tag{9}$$

$$\Psi_a^{\max}(z)=A\cos\left[\alpha\left[z-\frac{a}{2}\right]\right],\quad \Psi_b^{\max}=B\sin\left[\beta\left[z+\frac{b}{2}\right]\right]\quad \text{for } V<E\ . \tag{10}$$

Following the same procedure as above, we obtain the maximum energy of every odd-index band:

$$\tan\left[\frac{a}{2\hbar}(2m_aE_{\max})^{1/2}\right]-\left[\frac{m_a}{m_b}\left[\frac{V}{E_{\max}}-1\right]\right]^{1/2}\coth\left[\frac{b}{2\hbar}[2m_b(V-E_{\max})]^{1/2}\right]=0\quad \text{for } V>E\ , \tag{11}$$

$$\tan\left[\frac{a}{2\hbar}(2m_aE_{\max})^{1/2}\right]-\left[\frac{m_a}{m_b}\left[1-\frac{V}{E_{\max}}\right]\right]^{1/2}\cot\left[\frac{b}{2\hbar}[2m_b(E_{\max}-V)]^{1/2}\right]=0\quad \text{for } V<E\ . \tag{12}$$

2. *Even-index bands ($n=2,4,6,\ldots$)*

For even-index bands, the minimum energy corresponds to $\cos\Phi=-1$ or $\Phi=\pm\pi$. Since Ψ_a is odd and Φ_a is $\pm\pi$, $\Phi_b=\Phi-\Phi_a$ is 0. Thus Ψ_b is even, and we can write

$$\Psi_a^{\min}(z)=A\sin\left[\alpha\left[z-\frac{a}{2}\right]\right],\quad \Psi_b^{\min}=B\cosh\left[\delta\left[z+\frac{b}{2}\right]\right]\quad \text{for } V>E\ , \tag{13}$$

$$\Psi_a^{\min}(z)=A\sin\left[\alpha\left[z-\frac{a}{2}\right]\right],\quad \Psi_b^{\min}=B\cos\left[\beta\left[z+\frac{b}{2}\right]\right]\quad \text{for} V<E\ . \tag{14}$$

Using the boundary condition and simplifying as above, we obtain the minimum energy of every even-index band:

$$\cot\left[\frac{a}{2\hbar}(2m_aE_{\min})^{1/2}\right]+\left[\frac{m_a}{m_b}\left[\frac{V}{E_{\min}}-1\right]\right]^{1/2}\tanh\left[\frac{b}{2\hbar}[2m_b(V-E_{\min})]^{1/2}\right]=0\quad \text{for } V>E\ , \tag{15}$$

$$\cot\left[\frac{a}{2\hbar}(2m_aE_{\min})^{1/2}\right]-\left[\frac{m_a}{m_b}\left[1-\frac{V}{E_{\min}}\right]\right]^{1/2}\tan\left[\frac{b}{2\hbar}[2m_b(E_{\min}-V)]^{1/2}\right]=0\quad \text{for } V<E\ . \tag{16}$$

The smallest solution of Eq. (15) corresponds to $n=2$, the next to $n=4$, etc. The band index corresponding to the smallest solution of Eq. (16) depends on how many bands are confined inside the well.

To find the maximum energy of every even-index band we note that $\cos\Phi$ is 1 or Φ is 0. Since Ψ_a is odd and Φ_a is $\pm\pi$, $\Phi_b=\Phi-\Phi_a$ is $\pm\pi$. Thus Ψ_b is odd. Hence, we can write the wave functions as

$$\Psi_a^{\max}(z)=A\sin\left[\alpha\left[z-\frac{a}{2}\right]\right],\quad \Psi_b^{\max}=B\sinh\left[\delta\left[z+\frac{b}{2}\right]\right]\quad \text{for } V>E\ , \tag{17}$$

$$\Psi_a^{\max}(z)=A\sin\left[\alpha\left[z-\frac{a}{2}\right]\right],\quad \Psi_b^{\max}=B\sin\left[\beta\left[z+\frac{b}{2}\right]\right]\quad \text{for } V<E\ . \tag{18}$$

Following the same procedure as above, we obtain the maximum energy of every even-index band:

$$\cot\left[\frac{a}{2\hbar}(2m_aE_{\max})^{1/2}\right]+\left[\frac{m_a}{m_b}\left[\frac{V}{E_{\max}}-1\right]\right]^{1/2}\coth\left[\frac{b}{2\hbar}[2m_b(V-E_{\max})]^{1/2}\right]=0 \quad \text{for } V>E\ , \tag{19}$$

$$\cot\left[\frac{a}{2\hbar}(2m_aE_{\max})^{1/2}\right]+\left[\frac{m_a}{m_b}\left[1-\frac{V}{E_{\max}}\right]\right]^{1/2}\cot\left[\frac{b}{2\hbar}[2m_b(E_{\max}-V)]^{1/2}\right]=0 \quad \text{for } V<E\ . \tag{20}$$

Even though formulas similar to Eqs. (7) and (19) have been previously derived by Masselink *et al.*,[11] their relationship to the Kronig-Penney model has not been clarified. In addition, they are not a complete formalism because they cannot yield the maximum energies of odd-index bands and minimum energies of even-index bands, and the corresponding envelope wave functions.

The question might arise why only one boundary condition at $z=0$ was used in developing the new formalism, whereas boundary conditions at both $z=0$ and $z=a$ were used to derive Eqs. (3) and (4). The explanation lies in the main difference between the two formalisms. Since the conventional formalism is concerned with all the energies from 0 to ∞, Eqs. (3) and (4) indicate that Φ $(=kd)$ can be any real value from 0 to 2π (for energies inside bands) or any complex value (for energies outside bands). Thus there are no definite parities of Ψ_a and Ψ_b and no symmetry relationship between $\Psi_a(0)$ and $\Psi_a(a)$ or $\Psi_b(-b)$ and $\Psi_b(0)$. Therefore, in Fig. 1, the boundary condition at $z=0$ and $z=a$ are different and both boundary conditions must be used. On the other hand, the new formalism is only concerned with the band-edge energies, at which Φ can be only 0 or $\pm\pi$. Thus Ψ_a and Ψ_b have definite parities. Since $\Psi_a(0)=\pm\Psi_a(a)$ and $\Psi_b(0)=\pm\Psi_d(a)$, the boundary condition at $z=0$, which determines the relationship between Ψ_a and Ψ_b, is identical to that at $z=a$. This is the reason we need only one boundary condition in developing the new formalism.

When b becomes sufficiently large for $V>E$, Eqs. (7) and (11) degenerate to

$$\tan\left[\frac{a}{2\hbar}(2m_aE)^{1/2}\right]-\left[\frac{m_a}{m_b}\left[\frac{V}{E}-1\right]\right]^{1/2}=0$$

for $n=1,3,5,\ldots$

and Eqs. (15) and (19) to

$$\cot\left[\frac{a}{2\hbar}(2m_aE)^{1/2}\right]+\left[\frac{m_a}{m_b}\left[\frac{V}{E}-1\right]\right]^{1/2}=0$$

for $n=2,4,6,\ldots$.

These results are, of course, identical to the single-well results.[13]

III. APPLICATION AND DISCUSSION

As an illustration of the application of the new formalism, we have calculated the electron energy subbands of a $GaAs/Al_xGa_{1-x}As$ superlattice with $x=0.5$, $a=100$ Å, and $b=25$ Å by using both the conventional formalism [Eqs. (3) and (4)] and the new formalism [Eqs. (5) to (20)]. We have also calculated the envelope wave functions using the new formalism.

Figure 2 shows the first five electron energy subbands. We have taken $\Delta E_g=0.476+0.125x+0.143x^2$ eV for $0.45<x<1$,[14] as the band-gap difference between GaAs and $Al_xGa_{1-x}As$ at room temperature; $m_a=0.067m_0$ and $m_b=(0.067+0.083x)m_0$,[15] where m_0 is the free electron mass, as the electron effective mass at well and barrier layers. We have assumed 65%:35% band offset ratio[11,16,17] between the conduction and valence band. Thus the barrier potential V is given as $0.65\Delta E_g=375$ meV. As shown in Fig. 2, the first three bands are confined inside the well and the remaining two bands are not. Curve (a) in Fig. 2 corresponds to the function in the left-hand side of Eqs. (7) and (8) for $E<V$ and $E>V$, respectively. This curve meets the E axis at 31, 268, and 684 meV. Since Eqs. (7) and (8) give the minimum energies of odd-index bands, these three values are the minimum energy of the first, third, and fifth subband, respectively. Curve (b) corresponds to the functions in the left-hand side of Eqs. (11) and (12). Obviously, it gives the maximum energy of the first, third, and fifth subband. Similarly, curves (c) and (d) correspond to the functions in the left-hand side of Eqs. (15) and (16), and (19) and (20), respectively.

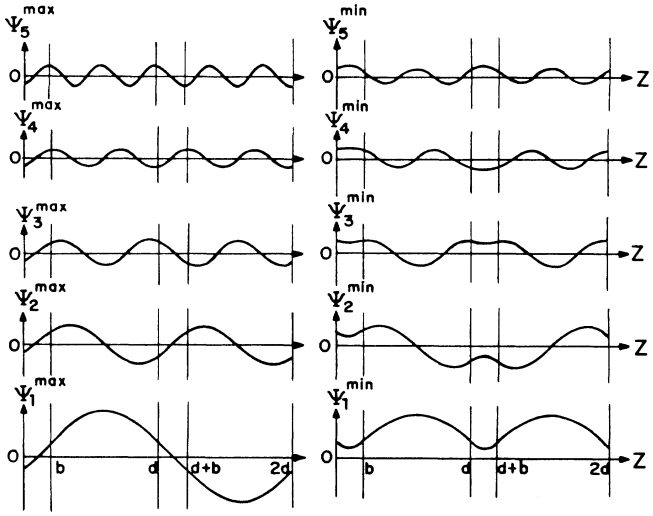

FIG. 3. Envelope wave functions corresponding to the edge energies of the first five subbands shown in Fig. 2. $\Psi_1^{\max}$ is the wave function corresponding to the maximum edge of the first subband, and $\Psi_1^{\min}$ is that corresponding to the minimum edge of the first subband, etc. $b=25$ Å is the barrier thickness; $a=d-b=100$ Å is the well thickness. The amplitude of the wave functions has arbitrary units.

They give the minimum and maximum energies of the second and fourth subband, respectively. All these curves are obtained from the new formalism. Curve (e) is obtained from the conventional formalism. It corresponds to the functions in the right-hand side of Eqs. (3) and (4) for $E < V$ and $E > V$, respectively. We can easily identify the first five subbands.

If we define $f(E)$ as the longitudinal axis of the curves (a)–(e), we note that curve (e) meets the $f(E)=1$ or -1 line at exactly the same points on the E axis as the minimum and maximum energies found from curves (a), (b), (c), and (d). This indicates that the energy bands found from the new formalism are identical to those found from the conventional formalism, as they must be. Even though we have plotted complete curves of functions in Eqs. (7), (8), (11), (12), (15), (16), (19), and (20) to find the subbands by the new formalism, usually it is not necessary. The energy bands can be easily found by simple numerical or graphical methods. Of course this formalism can also be used for bulk materials with $m_a = m_b$.

In Fig. 3 the envelope wave functions are presented, which correspond to the minimum and maximum energies of the first five subbands of the superlattice in Fig. 2. These wave functions have been found by using the minimum and maximum energy of each band in calculating α, β, and δ; also the boundary condition $\Psi_a(0)=\Psi_b(0)$ is applied to Eqs. (5), (6), (9), (10), (13), (14), (17), and (18), thus eliminating A or B. Although these wave functions are not normalized, $P_b = I_b/(I_a + I_b)$, where $I_a = \int_0^a |\Psi_a|^2 dz$ and $I_b = \int_{-b}^0 |\Psi_b|^2 dz$, gives the probability to find an electron at a barrier layer. The calculated values of P_b for this superlattice have been found to be 5.7%, 12%, 25%, 38%, and 43% for minimum energy of the first five bands, and 1.3%, 5.3%, 8%, 13%, and 18% for maximum energy of the first five bands. They are an increasing function of n, because electrons become more energetic with increasing n and are more probable to leak to the barriers. $P_b^{\min}$ for $\Psi_b^{\min}$ is larger than $P_b^{\max}$ for $\Psi_b^{\max}$ of the same band, because $\Psi_b^{\min}$ has even parity and $\Psi_b^{\max}$ has odd parity.

We observe another general property of the envelope wave functions in wells and barriers of superlattices: When $E < V$, wave functions at the wells, corresponding to both $E_{\min}$ and $E_{\max}$ of the nth subband, have $n-1$ zeros (meet z axis $n-1$ times). Those at the barriers have 0 (for $E_{\max}$) or 1 (for $E_{\min}$) zero. When $E > V$, wave functions at the wells still have $n-1$ zeros; those at the barriers have a different number of zeros for different b, ranging from 0 for small b, to infinity for infinitely large b. In Fig. 3, however, we see only 0 or 1 zero inside the barrier, because the barrier is sufficiently thin to have only 0 or 1 zero.

In conclusion, we can calculate both the energy bands and the wave functions corresponding to the edge energies of each band, of superlattices or bulk materials, using the new formalism of the Kronig-Penney model. Moreover, the calculation of energy bands can be done more easily by the new formalism than by the conventional formalism. The new formalism is very useful for the analysis of superlattices and application to device designs.

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