Envelope-Function Equation and Motion of Wave Packet in a Semiconductor Superlattice Structure

Byoung-Whi Kim, Yong Il Jun, and Hee Bum Jung

CONTENTS

ABSTRACT

We present a new description of envelope-function equation of the superlattice (SL). The SL wave function and corresponding effective-mass equation are formulated in terms of a linear combination of Bloch states of the constituent material with smaller band gap. In this envelope-function formalism, we review the fundamental concept on the motion of a wave packet in the SL structure subjected to steady and uniform electric fields $\mathbf{F}$. The review confirms that the average of SL crystal momentums $\mathbf{K} = (k_x, k_y, q)$, where (k_x, k_y) are bulk inplane wave vectors and q SL wave vector, included in a wave packet satisfies the equation of motion $\langle \mathbf{K} \rangle = \langle \mathbf{K} \rangle_0 + \mathbf{F}t/\hbar$; and that the velocity and acceleration theorems provide the same type of group velocity and definition of the effective mass tensor, respectively, as in the Bulk. Finally, Schlosser and Marcus's method for the band theory of metals has been used by Altarelli to include the interface-matching condition in the variational calculation for the SL structure in the multi-band envelope-function approximation. We re-examine this procedure more thoroughly and present variational equations in both general and reduced forms for SLs, which agrees in form with the proposed envelope-function formalism. As an illustration of the application of the present work and also for a brief investigation of effects of band-parameter difference on the subband energy structure, we calculate by the proposed variational method energies of non-strained GaAs/$Al_{0.32}Ga_{0.68}$As and strained $In_{0.63}Ga_{0.37}As/In_{0.73}Ga_{0.27}As_{0.58}P_{0.42}$SLs with well/barrier widths of 60 $\mathring{\mathrm{A}}$/500 $\mathring{\mathrm{A}}$ and 30 $\mathring{\mathrm{A}}$/30 $\mathring{\mathrm{A}}$, respectively.

I. INTRODUCTION

The flexibility in semiconductor superlattices (SLs) electronic properties makes them useful in many technological applications, including semiconductor lasers, electro-optical modulators, nonlinear optical devices, and infrared photodetectors. For this reason, after the pioneering work of Esaki and Tsu [1], a significant number of research results have been reported and much understanding of the fundamental physics has been obtained on this fascinating structure [2]-[14].

Among the previous theoretical studies on the electronic properties of semiconductor SLs, within the effective-mass $\mathbf{k}\cdot\mathbf{p}$ approximation, White and Sham [4] and Bastard [5] proposed theories with a two-band model comprising the conduction and light-hole bands. Altarelli [6] proposed a three-band (the conduction band and the heavy- and light-hole bands) $\mathbf{k}\cdot\mathbf{p}$ formalism for a self-consistent electronic structure calculation. In those approaches above, the zone center Bloch functions and band parameters are taken to be identical for the constituent materials. Pötz *et al.* [8] proposed an envelope-function approach to describe semiconductor heterogeniety in space. In their model a set of coupled differential equations is set up in the envelope-function approximation, and then decoupled nonlinear (in energy) differential equations are obtained by ignoring terms higher than second order in d/dz. Energies are determined by solving these with interface matching conditions for the envelopes. D. L. Smith and C. Mailhiot [9] presented a complete theory of SLs. In their work, a single basis set for constituent materials, obtained using the empirical pseudopotentials, is used to describe a zone-center of a reference virtual system whose lattice constant is the average of the lattice constants of the constituent materials. Near-in energy states are treated in Lowdin perturbation theory [15] with $\mathbf{k}\cdot\mathbf{p}$ operator and the difference between the material pseudopotential and the reference pseudopotential as the perturbation. They also presented a rigorous analysis on matching conditions at SL interfaces. Although, as compared with previous work, their theory provides a very accurate and rigorous description of the SL, in which the SL symmetry is treated more properly so that band-splitting and -mixing features are revealed correctly, one disadvantage could be in the implementation of numerical computations: it requires computations for reference zone-center energies, cell-periodic functions, and $\mathbf{k}\cdot\mathbf{p}$ momentum matrix elements from the zone-center states, to establish the SL eigenvalue equation, which then has to be solved to finally obtain subband energy dispersion and SL wave vectors. On the other hand, in the bulk semiconductors, $\mathbf{k}\cdot\mathbf{p}$ theory is particularly effective at describing states near the conduction- and valence-band edges. Thus it is natural to attempt applying the $\mathbf{k}\cdot\mathbf{p}$ theory to the SL in considering it as a

perfectly periodic structure. On this line, Johnson *et al.* [11] proposed a simpler approach that is easy to implement numerical computations without large-scale computation and yields reliable results for SL properties. The theory is based on closed analytic calculations of the SL states at wave vector $\mathbf{K} = (k_t, q) = 0$, where $k_t = (k_x, k_y)$ are inplane bulk wave vectors and q SL wave vector. Then the SL $\mathbf{K}\cdot\mathbf{p}$ theory is employed to yield the SL band structure at finite $\mathbf{K}$ states. In this theory the SL wave function is formed by a linear combination of zone-center Bloch functions, which are assumed to be identical for both materials.

In the treatment of the band parameter difference (BPD) of constituent materials in most previous work, Hamiltonians in each layer are solved to yield "local" eigenvalues and functions. True eigenvalues and functions of a given SL system are then calculated by applying the SL translational symmetry and matching of "local" envelope functions and current-continuity at the interfaces. Thus this approach considers the SL as being formed with two different eigensystems. In this paper we propose a different approach, in which the SL effective-mass equation is solved as a whole. In this approach, the differences in the bulk Bloch functions as well as the band parameters enter into a form of SL potential. The symmetry of SL and the current-continuity at the interfaces are implicitly taken into account through the order in perturbation theory at which the bulk Bloch function at $\mathbf{k}$ is obtained in terms of the zone-center Bloch functions. In the usual envelope-function approximation, the present description is simplified significantly.

The motion of a wave packet in a crystalline solid subjected to steady and uniform electric fields has been well established. The average of crystal momentums $\mathbf{k}$ included in a wave packet satisfies the equation of motion $\langle\mathbf{k}\rangle = \langle\mathbf{k}\rangle_0 + \mathbf{F}t/\hbar$, where $\mathbf{F}$ is the external electric field; and the velocity and acceleration theorems provide the group velocity of the packet $\mathbf{v}_g = (1/\hbar)\nabla_{\mathbf{k}}E(\mathbf{k})$ and definition of the effective mass tensor, respectively. These frame a fundamental concept of effective-mass representation for crystalline solids. It is natural to consider that these are applicable to SLs due to their perfectly periodic structure, because physics associated with periodic structure of crystalline solid provides that the additional periodic perturbation of SL yields a new crystal momentum q associated with the SL direction (Bloch theory), and indicates that same formalisms for bulk periodic solids are applicable to the SL structure including the $\mathcal{E}(q)$ dispersion and the $\mathbf{K}\cdot\mathbf{p}$ theory. Also, in the presence of applied electric field, the quasiparticle picture of carriers along the SL direction can be used to characterize electronic properties of SLs, if the voltage drop across each period is less than the subband energy width so that the Bloch-like structure remains to some extent.

Many of theories used to explain carrier

transport properties along the SL direction have assumed the quasiparticle picture of carriers [1]-[3]. Esaki and Tsu [1] used a simplified path integration method to obtain a relation between the applied field F and the average drift velocity v_d in the SL direction. In obtaining the solutions for the drift velocity, they used the SL equation of motion $\hbar\partial q/\partial t = eF$. Lebwohl and Tsu [2] derived and used more general expression for the average current in the SL direction with constant electric field applied in that direction. They used the SL effective-mass velocity $\partial v_z/\hbar\partial q$ and assumed an energy-independent isotropic relaxation time for the scattering term in the Boltzmann equation. The dispersion relation and effective masses of the SL, $\mathcal{E}(q) = \hbar^2 q^2/2m_z^*$, have been discussed in detail by Bastard [5]. As discussed before, Johnson *et al.* [11] obtained the electronic structure and optical properties of III-V and II-VI semiconductor SLs using an SL effective-mass-representation formalism in the envelope-function approximation [6], [7]. In this paper, we review these fundamental concepts of the motion of a wave packet and the velocity and acceleration theorems in the structure of SL subjected to steady and uniform electric fields.

Among the many computation methods [16] to obtain energies and wave functions of the quantum well and SL systems, the variational method has unique advantages: in the numerical computation point of view, the method provides "stable" result[1] for both confined and virtual eigenstates when the trial functions are set up properly; it also provides easier ways to implement self-consistent computations when Hartree and exchange-correlation interactions are included. There has been proposed an efficient variational scheme to solve the multi-band envelope-function equation for SLs, where interface-matching conditions are taken into account [6]. This method was developed by extending the method by Schlosser and Marcus (SM) [17] in the band theory of metals. However, detailed description of the procedure has not been presented. We re-examine the procedure more thoroughly and present variational equations in both general and reduced forms. We show that, when envelope functions are expanded by the same kind of basis functions for both material layers, the current-continuity condition does not explicitly enter into the final equation; instead, BPD acts as an SL potential in the larger band-gap material region (material B). This feature agrees with the result of the new envelope-function equation, which will be proposed in this paper.

As an illustration of application of the present approach, and also to briefly investigate the importance of taking into account

[1]In the multiband transfer matrix method, for example, the accuracy in determining eigenvalues (energies) from vanishing determinant of the resultant transfer matrix reduces in general when energies become larger and closer to the barrier height.

the BPD, we calculate subband energies of SLs with well/barrier thicknesses of 60 Å/500 Å and 30 Å/30 Å both for non-strained GaAs/AlGaAs and strained InGaAs/InGaAsP SLs. Comparisons are made between the present results and those reported previously. A brief remark is made on the effects of BPD on the subband energy structure for the two types of model SLs above.

The paper is organized in the following way. Section II presents the new description of SL equation. Section III reviews the motion of a wave packet and related velocity and acceleration theorems in the SL structure. In Sec. IV we review the variational procedure for the SL structure based on the SM's method. Sample calculations are also presented in this section. Finally, conclusions are drawn in Sec. V.

II. SUPERLATTICE EFFECTIVE-MASS EQUATION

In this section we present an effective-mass envelope-function equation for SLs. The quantum states of SL can be expressed by a linear combination of $|v,\mathbf{k}\rangle^A = u^A_{v,\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$, where v is band index in the bulk, $u^A_{v,\mathbf{k}}(\mathbf{r})$ cell periodic function of the bulk for material type A (material with smaller band gap) at quantum state $\mathbf{k}=(\mathbf{k}_t,k_z)$:

$$|\mathbf{K}_t,n,q\rangle = \sum_{v',\mathbf{k}'_t,k'_z} a(\mathbf{k}_t,n,q;v',\mathbf{k}'_t,k'_z)|v',\mathbf{k}'\rangle^A, \tag{1}$$

where n is SL subband index and q is the wave vector associated with the SL direction (z-direction). Note that in Eq. (1) we employ a basis set of material A to describe the states for both the constituent materials.

Upon substituting Eq. (1) into the SL Schrödinger equation of

$$\left[H_0^A+V^A\theta_z^A+H_0^B+V^B\theta_z^B\right]|\mathbf{k}_t,n,q\rangle = \mathcal{E}|\mathbf{k}_t,n,q\rangle, \tag{2}$$

where the function $\theta_z^{A(B)}$ is unity in the material A (B) region and zero elsewhere, H_0 is the free electron kinetic energy operator, $V^{A(B)}(\mathbf{r})$ is the cell-periodic lattice potential of material A(B) including the Hartree and exchange-correlation potentials [14]. Operating ${}^A\langle v,0|e^{-i\mathbf{k}\cdot\mathbf{r}}$ on Eq. (2) from the left, we obtain

$$\begin{aligned}
&\mathcal{E}a(\mathbf{k}_t,n,q;v,\mathbf{k}_t,k_z)\\
&= {}^A\langle v,0|e^{-i\mathbf{k}\cdot\mathbf{r}}\left[H_0^A+V^A+H_0^B-H_0^A\theta_z^B+V^B-V^A\theta_z^B\right]\sum_{\mathbf{k}'_t,k'_z,v'}|v',\mathbf{k}'\rangle^A a(\mathbf{k}_t,n,q;v',\mathbf{k}'_t,k'_z)\\
&= \sum_{v',\mathbf{k}'_t,k'_z} H_{vv'}(\mathbf{k},\mathbf{k}')a(\mathbf{k}_t,n,q;v',\mathbf{k}'_t,k'_z) + \sum_{v',\mathbf{k}'_t,k'_z} W_{vv'}(\mathbf{k},\mathbf{k}')a(\mathbf{k}_t,n,q;v',\mathbf{k}'_t,k'_z),
\end{aligned} \tag{3}$$

where the "fundamental" term $H_{vv'}$ and the "SL potential term" $W_{vv'}$ are defined, respectively, as

$$H_{vv'}(\mathbf{k},\mathbf{k}') = \langle v,0|e^{-i\mathbf{k}\cdot\mathbf{r}}H_0^A + V^A|v',\mathbf{k}'\rangle_A \cong \left(\mathcal{E}_{v,0}^A + \frac{\hbar^2 k^2}{2m_0}\right)\delta_{vv'}\delta_{\mathbf{k},\mathbf{k}'} + L'_{vv'}\delta_{\mathbf{k},\mathbf{k}'}, \tag{4}$$

$$\begin{aligned} W_{vv'}(\mathbf{k},\mathbf{k}') &= \langle v,0|e^{-i\mathbf{k}\cdot\mathbf{r}}H_0^B + V^B\theta_z^B|v',\mathbf{k}'\rangle_A - \langle v,0|e^{-i\mathbf{k}\cdot\mathbf{r}}H_0^A + V^A\theta_z^B|v',\mathbf{k}'\rangle_A \\ &\cong \int dz e^{i(k_z'-k_z)z}\left[\sum_l (c_{v'}^l)^* c_v^l \left(\mathcal{E}_{l,0}^B + \frac{\hbar^2 k'^2}{2m_0}\right) - \left(\mathcal{E}_{v,0}^A + \frac{\hbar^2 k'^2}{2m_0}\right)\theta_z^B\delta_{\mathbf{k}_t,\mathbf{k}_t'}\right] \\ &\quad + \int dz e^{i(k_z'-k_z)z}\sum_{l,l'}(c_{v'}^{l'})^* c_v^l L_{ll'}^B - L_{vv'}^A\theta_z^B\delta_{\mathbf{k}_t,\mathbf{k}_t'}. \end{aligned} \tag{5}$$

Here overlap coefficient c_v^l is defined as

$$c_v^l = {}^B\langle l,0|v,0\rangle^A, \tag{6}$$

and $L_{vv'}$ replaces the $\mathbf{k}\cdot\mathbf{p}$ perturbation terms [18] with the Luttinger parameters [19] introduced to compensate the truncation beyond those bands of interest in the perturbation description:

$$L_{vv'}(\mathbf{k}) \equiv \frac{\hbar}{m_0}\langle v,0|\mathbf{k}\cdot\mathbf{p}|v',0\rangle + \left(\frac{\hbar}{m_0}\right)^2 \sum_{N\neq J} \frac{\langle v,0|\mathbf{k}\cdot\mathbf{p}|N,0\rangle\langle N,0|\mathbf{k}\cdot\mathbf{p}|v',0\rangle}{\mathcal{E}_{v,0} - \mathcal{E}_{N,0}}, \tag{7}$$

where J consists of the primary bands. Detailed algebraic steps taken to reach Eqs. (4) and (5) are presented in Appendix A. Taking the Fourier transform on Eq. (3) with respect to k_z' , we obtain an expression for the one-particle SL effective-mass equation:

$$\mathcal{E}\Psi(v,\mathbf{k}_t,n,q;z) = \sum_{v'}[H_{vv'}(\mathbf{k}_t,-i\partial_z) + W_{vv'}(\mathbf{k}_t,-i\partial_z)]\Psi(v',\mathbf{k}_t,n,q;z). \tag{8}$$

Obviously, the accuracy of the method depends on the availability of the overlap coefficients $c_{v'}^v$. These quantities can be computed once and for all for given constituent materials. Although taking the coefficients into consideration yields more exact description of SL properties including the SL symmetry, a model for simple computations can be established by assuming that the coefficient can be approximated as $c_v^l = \delta_{v,l}$, while keeping the BPD in the equation:

$$W_{vv'}(\mathbf{k},\mathbf{k}') \cong \int dz e^{i(k_z'-k_z)z}\left(\mathcal{E}_{v,0}^B - \mathcal{E}_{v,0}^A + L_{vv'}^B - L_{vv'}^A\right)\theta_z^B\delta_{\mathbf{k}_t,\mathbf{k}_t'}. \tag{9}$$

This assumption has been used in the usual envelope-function approximation. In Section IV, it will be shown that the same result can be obtained through considering a variational procedure in the envelope-function approximation. We note that, when $\mathbf{k}_t = 0$, the multiband equation becomes decoupled and each one has the potential of

$$W_{vv'}(k_z,k_z') = \int dz e^{i(k_z'-k_z)z}\left(\mathcal{E}_{v,0}^B - \mathcal{E}_{v,0}^A\right)\theta_z^B; \tag{10}$$

that is, difference of the zone-center-energy becomes a potential barrier as in the Kronig-Penney model.

III. MOTION OF WAVE PACKET IN THE SUPERLATTICE

In this section we review the velocity and acceleration theorems and the motion of wave packets in the SL structure by following the usual procedure used in deriving these for the bulk crystalline solids [20].

1. Velocity and Acceleration

The energy of a quantum state (k_t', n', q') can be expanded to first order of differences in in-plane and SL wave vectors in terms of the energy of a nearby quantum state $(\mathbf{k}_t, n', q)$ in the same subband n':

$$\mathcal{E}(\mathrm{k}_t', n', q') = \mathcal{E}(\mathbf{k}_t, n', q) + (\mathrm{k}_t' - \mathbf{k}_t)\cdot\nabla_{\mathbf{k}_t}\mathcal{E}(\mathbf{k}_t, n', q) + (q'-q)\nabla_q\mathcal{E}(\mathbf{k}_t, n', q). \tag{11}$$

As discussed in the previous section, the SL envelope function can be expressed as

$$\Psi(v, \mathbf{k}_t, n, q; z) = \sum_{k_z} a(v, \mathbf{k}_t, n, q; k_z) e^{ik_z z} = \varphi(v, \mathbf{k}_t, n, q; z) e^{iqz}, \tag{12}$$

where the periodic part φ satisfies $\varphi(v,\ \mathbf{k}_t, n, q; z) = \varphi(v, \mathbf{k}_t, n, q; z+d)$.

The wave packet of a particle in the SL can be expressed by a linear combination of the SL eigenfunctions:

$$\begin{aligned}\Psi(\mathbf{r}, t) &= \sum_{\mathrm{k}_t', n', q'} A(\mathrm{k}_t', n', q', t)\langle \mathbf{r}|\mathrm{k}_t', n', q'\rangle = \sum_{\mathrm{k}_t', n', q'} A(\mathrm{k}_t', n', q')\langle \mathbf{r}|\mathrm{k}_t', n', q'\rangle e^{-i\mathcal{E}(\mathrm{k}_t', n', q')t/\hbar}. \\ &= \sum_{\mathrm{k}_t', n', q'} A(\mathrm{k}_t', n', q') \sum_{v, k_z'} a(v, \mathrm{k}_t', n', q'; k_z')\langle \mathbf{r}|v, \mathbf{k}'\rangle e^{-i\mathcal{E}(\mathrm{k}_t', n', q')t/\hbar}.\end{aligned} \tag{13}$$

Using the velocity operator $v_z = (i/\hbar)[Hz - zH]$, the group velocity of the wave packet can be obtained by

$$\begin{aligned}\langle v_z\rangle &= \int d^3r \Psi^*(\mathbf{r}, t) v_z \Psi(\mathbf{r}, t) \\ &= \sum_{\mathbf{k}_t n q} \sum_{\mathrm{k}_t' n' q'} A^*(\mathbf{k}_t, n, q, t) A(\mathrm{k}_t', n', q', t)\, \langle \mathbf{k}_t, n, q|(i/\hbar)(Hz - zH)|\mathrm{k}_t', n', q'\rangle \\ &= \sum_{\mathbf{k}_t, n, q} A^*(\mathbf{k}_t, n, q, t) \left(\frac{1}{\hbar}\frac{\partial}{\partial q}\mathcal{E}(\mathbf{k}_t, n, q)\right) A(\mathbf{k}_t, n, q, t) \\ &\quad + \sum_{\mathbf{k}_t, q, n, n'} A^*(\mathbf{k}_t, n, q, t) A(\mathbf{k}_t, n', q, t) \frac{i}{\hbar}\left(\mathcal{E}(\mathbf{k}_t, n, q) X_{nn'} + Y_{nn'} - X_{nn'} + Y_{nn'})\mathcal{E}(\mathbf{k}_t, n', q)\right),\end{aligned} \tag{14}$$

where

$$X_{nn'} = \sum_{v,v'} F^{(0)}_{vv'} \int e^{i(q'-q)z}\varphi^*(v,\mathbf{k}_t,n,q;z)\varphi(v',\mathbf{k}_t,n',q';z)dz, \tag{15}$$

$$Y_{nn'} = -i \sum_{v} \int dz \left(\frac{\partial}{\partial q}\varphi^*(v,\mathbf{k}_t,n,q;z)\right) \varphi(v,\mathbf{k}_t,n',q;z), \tag{16}$$

$F^{(0)}_{vv'}$ is defined in Eq. (B7), and detailed algebraic steps taken to obtain the above result are presented in Appendix B.

The first term on the right side of Eq. (14) is associated with the motion of a particle in a given subband, and the second term with transitions between bands which comprises the phenomena of tunneling. Tunneling between different subbands becomes important only for strong fields. As we are concerned with the transport of carriers through a given subband under a weak field, we neglect the off-diagonal terms. In this case the average velocity becomes

$$\langle v_z\rangle = \sum_{\mathbf{k}_t,n,q} A^*(\mathbf{k}_t,n,q,t)\left(\frac{1}{\hbar}\frac{\partial}{\partial q}\mathcal{E}(\mathbf{k}_t,n,q)\right) A(\mathbf{k}_t,n,q,t), \tag{17}$$

which indicates that the velocity operator can be expressed in the SL crystal momentum representation as

$$v_z(q)\big|_{\mathbf{k}_t,n} = \frac{1}{\hbar}\frac{\partial}{\partial q}\mathcal{E}(\mathbf{k}_t,n,q). \tag{18}$$

It can be easily shown that Eq. (17) can be generalized to an arbitrary velocity vector by using the velocity operator $(i/\hbar)[H\mathbf{r}-\mathbf{r}H]$:

$$\langle \mathbf{v}\rangle = \sum_{\mathbf{k}_t,n,q} A^*(\mathbf{k}_t,n,q,t)\left(\frac{1}{\hbar}\nabla_{\mathbf{K}}\mathcal{E}(\mathbf{k}_t,n,q)\right) A(\mathbf{k}_t,n,q,t). \tag{19}$$

The time rate of change of the average velocity under the electric field along the SL direction is given by

$$\begin{aligned}\frac{d\langle \mathbf{v}\rangle}{dt} &= \frac{1}{\hbar}\sum_{\mathbf{k}_t,n,q} \nabla_{\mathbf{K}}\mathcal{E}(\mathbf{k}_t,n,q)\left(\frac{\partial A^*(\mathbf{k}_t,n,q,t)}{\partial t}A(\mathbf{k}_t,n,q,t) + A^*(\mathbf{k}_t,n,q,t)\frac{\partial A(\mathbf{k}_t,n,q,t)}{\partial t}\right)\\ &= -\frac{1}{\hbar}\frac{F}{\hbar}\sum_{\mathbf{k}_t,n,q} \nabla_{\mathbf{K}}\mathcal{E}(\mathbf{k}_t,n,q)\left(\frac{\partial A^*(\mathbf{k}_t,n,q,t)}{\partial q}A(\mathbf{k}_t,n,q,t) + A^*(\mathbf{k}_t,n,q,t)\frac{\partial A(\mathbf{k}_t,n,q,t)}{\partial q}\right)\\ &= \frac{F}{\hbar^2}\sum_{\mathbf{k}_t,n,q} A^*(\mathbf{k}_t,n,q,t)\left(\frac{\partial}{\partial q}\nabla_{\mathbf{K}}\mathcal{E}(\mathbf{k}_t,n,q)\right) A(\mathbf{k}_t,n,q,t),\end{aligned} \tag{20}$$

where we use Eq. (26) and an integration by part. This result can be associated with an acceleration at a state of $(\mathbf{k}_t, n, q)$ as

$$\vec{\alpha}_z(\mathbf{k}_t, n, q) = \frac{F}{\hbar^2}\frac{\partial}{\partial q}\nabla_{\mathbf{K}}\mathcal{E}(\mathbf{k}_t, n, q). \tag{21}$$

In the case of an arbitrary directed field, it is generalized to

$$\vec{\alpha}_z(\mathbf{k}_t, n, q) = \frac{1}{\hbar^2}(\mathbf{F}\cdot\nabla_{\mathbf{K}})\nabla_{\mathbf{K}}\mathcal{E}(\mathbf{k}_t, n, q). \tag{22}$$

Finally, the reciprocal effective mass tensor in the SL can be obtained by comparing Eq. (22) with

$$\alpha_j(\mathbf{k}_t, n, q) = \sum_i \frac{1}{m^*_{ji}}F_i. \tag{23}$$

2. Motion of Wave Packet

Applying the form of the wave packet in Eq. (13) to the time-dependent Schrödinger equation, $(H_0+U)\psi(\mathbf{r},t) = i\hbar(\partial/\partial t)\psi(\mathbf{r},t)$, where H_0 is the SL Hamiltonian and U is an external potential ($U=-Fz$ for the electric field along the SL direction), the expansion coefficient A satisfies the time-dependent Schrödinger equation in the crystal momentum representation

$$(H_0+U)\sum_{\mathbf{k}'_t,n',q'} A(\mathbf{k}'_t,n',q',t)|\mathbf{k}'_t,n',q'\rangle = i\hbar\frac{\partial}{\partial t}\sum_{\mathbf{k}'_t,n',q'} A(\mathbf{k}'_t,n',q',t)|\mathbf{k}'_t,n',q'\rangle. \tag{24}$$

Operating $\langle\mathbf{k}_t,n,q|$ on Eq. (24) from the left, we obtain

$$\left[\mathcal{E}(\mathbf{k}_t,n,q) - i\hbar\frac{\partial}{\partial t}\right]A(\mathbf{k}_t,n,q,t) - F\sum_{\mathbf{k}'_t,n',q'}\langle\mathbf{k}_t,n,q|z|\mathbf{k}'_t,n',q'\rangle A(\mathbf{k}'_t,n',q',t) = 0$$

or

$$\left[\mathcal{E}(\mathbf{k}_t,n,q) - iF\frac{\partial}{\partial q} - i\hbar\frac{\partial}{\partial t}\right]A(\mathbf{k}_t,n,q,t) - F\sum_{n'}\left[X_{nn'}+Y_{nn'}\right]A(\mathbf{k}_t,n',q',t) = 0. \tag{25}$$

We note that for a weak field we can ignore the off-diagonal terms as discussed previously, and in this case it becomes

$$\left[\mathcal{E}(\mathbf{k}_t,n,q) - iF\frac{\partial}{\partial q} - i\hbar\frac{\partial}{\partial t}\right]A(\mathbf{k}_t,n,q,t) = 0. \tag{26}$$

If we multiply Eq. (26) by $A^*(\mathbf{k}_t, n, q, t)$, subtract from the resulting equation its complex conjugate, and sum on the subband index n, the terms involving the X and Y disappear on the summation. This follows because $X^*_{nn'} = X_{n'n}$ and $Y^*_{nn'} = Y_{n'n}$. We then obtain

$$\left(iF\frac{\partial}{\partial q} + i\hbar\frac{\partial}{\partial t}\right)\sum_n |A(\mathbf{k}_t, n, q, t)|^2 = 0. \tag{27}$$

The general solution of this equation is

$$\sum_n |A(\mathbf{k}_t, n, q, t)|^2 = G(\mathbf{k}_t, q - Ft/\hbar). \tag{28}$$

The average of wave vectors $\mathbf{K}$ contained in Ψ (the centroid of the wave packet) is defined to be

$$\langle \mathbf{K} \rangle = \sum_n \int |A(\mathbf{k}_t, n, q, t)|^2 \mathbf{K}\, d\mathbf{K}. \tag{29}$$

Only the z component is of interest as only it is affected by the field:

$$\begin{aligned}
\langle q \rangle &= \sum_n \int |A(\mathbf{k}_t, n, q, t)|^2 q\, dq \\
&= \int q G(\mathbf{k}_t, q - \frac{Ft}{\hbar}) dq = \int q \left(1 - \frac{Ft}{\hbar}\frac{\partial}{\partial q} + \frac{1}{2!}\left(\frac{Ft}{\hbar}\right)^2 \left(\frac{\partial}{\partial q}\right)^2 + \cdots\right) G(\mathbf{k}_t, q)\, dq \\
&= \int q G(\mathbf{k}_t, q) dq + \frac{Ft}{\hbar}\int G(\mathbf{k}_t, q) dq - \frac{1}{2!}\left(\frac{Ft}{\hbar}\right)^2 \int \frac{\partial}{\partial q} G(\mathbf{k}_t, q) dq + \cdots = \langle q \rangle_0 + Ft/\hbar,
\end{aligned} \tag{30}$$

because $\int_{-\infty}^{+\infty} G(\mathbf{k}_t, q) dq = 1$ from the normalization of wave function and

$$qG(\mathbf{k}_t, q)\Big|_{-\infty}^{+\infty} = q\frac{\partial}{\partial q} G(\mathbf{k}_t, q)\Big|_{-\infty}^{+\infty} = \cdots = 0, \tag{31}$$

where $\langle q \rangle_0$ is the location of the centroid at $t = 0$. This immediately leads to

$$\hbar\frac{\partial}{\partial t}\langle q \rangle = F. \tag{32}$$

The review presented in this section confirms that the SL crystal momentum q's are well-defined quantum numbers with which energy structure and motion of a particle under the external field can be described. It is also confirmed that particles in the SL can be treated as quasi free particles with corresponding effective masses. Therefore, some characteristic features of the transport property can be qualitatively taken through examining the effective masses: for example, the infrared photodetectors with p-type GaAs/AlGaAs SLs shows a lower dark current as the effective masses of heavy-hole minibands along the growth direction are heavier in general than those of conduction-band subbands [14].

IV. VARIATIONAL PROCEDURE FOR THE SUPERLATTICE STRUCTURE

In this section, we review the variational procedure based on the SM's method [17] to solve the multi-band effective-mass envelope-function equation for SLs. An explicit review on the current operator for envelope-functions is presented in Appendix C.

A variational form in the envelope-function representation for the present problem can be established by replacing the normal derivative operator ∂_n in Eq. (C9) [see also Eq. (A1.1) in Ref. 17] by the current operator J_z:

$$\mathcal{E}\left(\int_{L_A} dz\Psi_A^*\Psi_A + \int_{L_B} dz\Psi_B^*\Psi_B\right) = \int_{L_A} dz\Psi_A^* H_A\Psi_A + \int_{L_B} dz\Psi_B^* H_B\Psi_B + \frac{1}{2}\left[\Psi_A^* J_z\Psi_A - \Psi_A J_z\Psi_A^*\right]_{z=z_0} - \left[\Psi_A^* J_z\Psi_B - \Psi_B J_z\Psi_A^*\right]_{z=z_0} + \left[\Psi_B^* J_z\Psi_A - \Psi_A J_z\Psi_B^*\right]_{z=z_0} - \left[\Psi_B^* J_z\Psi_B - \Psi_B J_z\Psi_B^*\right]_{z=z_0}, \quad (33)$$

where $L_{A(B)}$ is the region of material A (B) along the z-direction.

When expanding the envelope functions by sets of plane waves as

$$\Psi_A = \sum_{l'} a_{l'} e^{i2\pi l' z/d}, \quad \Psi_A^* = \sum_{l} a_l^* e^{-i2\pi l z/d}, \quad \Psi_B = \sum_{l'} b_{l'} e^{i2\pi l' z/d}, \quad \text{and} \quad \Psi_B^* = \sum_{l} b_l^* e^{-i2\pi l z/d}, \quad (34)$$

where we consider the four expansion coefficients, $a_l^*, a_{l'}, b_l^*$, and $b_{l'}$, as being independent for the time being (which can be so when the envelope functions are expanded by different kinds of basis functions for different material regions), and differentiating the resultant equation with respect to a_l^* and b_l^*, we have, respectively,

$$\mathcal{E}\sum_{l'} a_{l'}\int_{L_A} dz e^{-i2\pi(l-l')z/d} = \sum_{l'} a_{l'}\int_{L_A} dz e^{-i2\pi lz/d} H_A e^{i2\pi l' z/d} + \frac{1}{2}\sum_{l'} a_{l'}\left[e^{-i2\pi lz/d} J_z^A e^{i2\pi l' z/d} - e^{i2\pi l' z/d} J_z^A e^{-i2\pi lz/d}\right]_{z=z_0} - \frac{1}{2}\sum_{l'} b_{l'}\left[e^{-i2\pi lz/d} J_z^B e^{i2\pi l' z/d} - e^{i2\pi l' z/d} J_z^A e^{-i2\pi lz/d}\right]_{z=z_0}, \quad (35)$$

$$\mathcal{E}\sum_{l'} b_{l'}\int_{L_B} dz e^{-i2\pi(l-l')z/d} = \sum_{l'} b_{l'}\int_{L_B} dz e^{-i2\pi lz/d} H_B e^{i2\pi l' z/d} - \frac{1}{2}\sum_{l'} b_{l'}\left[e^{-i2\pi lz/d} J_z^B e^{i2\pi l' z/d} - e^{i2\pi l' z/d} J_z^B e^{-i2\pi lz/d}\right]_{z=z_0} - \frac{1}{2}\sum_{l'} a_{l'}\left[e^{-i2\pi lz/d} J_z^A e^{i2\pi l' z/d} - e^{i2\pi l' z/d} J_z^B e^{-i2\pi lz/d}\right]_{z=z_0}, \quad (36)$$

These, respectively, can be written in matrix form as

$$\mathcal{E}\mathbf{D}^A\mathbf{a} = \mathbf{H}^A\mathbf{a} + \frac{1}{2}\left[\mathbf{J}^A(z_0) - \bar{\mathbf{J}}^A(z_0)\right]\mathbf{a} - \frac{1}{2}\left[\mathbf{J}^B(z_0) - \bar{\mathbf{J}}^A(z_0)\right]\mathbf{b}, \quad (37)$$

$$\mathcal{E}\mathbf{D}^B\mathbf{b} = \mathbf{H}^B\mathbf{b} - \frac{1}{2}\left[\mathbf{J}^B(z_0) - \bar{\mathbf{J}}^B(z_0)\right]\mathbf{b} + \frac{1}{2}\left[\mathbf{J}^A(z_0) - \bar{\mathbf{J}}^B(z_0)\right]\mathbf{a}, \quad (38)$$

Here **a** and **b** are column vectors consisting of a_l and b_l, respectively, and matrices above are

$$D^S_{ll'} = \frac{1}{d}\int_{L_S} dz e^{-i2\pi(l-l')z/d}, H^S_{ll'} = \frac{1}{d}\int_{L_S} dz e^{-i2\pi lz/d} H_s e^{i2\pi l'z/d},$$
$$J^S_{ll'}(z_0) = \frac{1}{d}\left[e^{-i2\pi lz/d} J^S_z e^{i2\pi l'z/d}\right]_{z=z_0}, \quad \text{and} \quad \bar{J}^S_{ll'}(z_0) = \frac{1}{d}\left[e^{i2\pi l'z/d} J^S_z e^{-i2\pi lz/d}\right]_{z=z_0}, \tag{39}$$

with $s = A, B$. Equations (37) and (38) can be combined as

$$\begin{pmatrix} \mathbf{D}^A & \\ & \mathbf{D}^B \end{pmatrix}\begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix} = \begin{pmatrix} \mathbf{H}^A & \\ & \mathbf{H}^B \end{pmatrix}\begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix} + \frac{1}{2}\begin{pmatrix} \mathbf{J}^A_{z_0} - \bar{\mathbf{J}}^A_{z_0} & -\mathbf{J}^B_{z_0} + \bar{\mathbf{J}}^A_{z_0} \\ \mathbf{J}^A_{z_0} - \bar{\mathbf{J}}^B_{z_0} & -\mathbf{J}^B_{z_0} + \bar{\mathbf{J}}^B_{z_0} \end{pmatrix}\begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix}. \tag{40}$$

However, Eq. (40) needs an additional term to meet the envelope-function continuity condition. Incorporation of this condition into this equation can be done more conveniently by considering $\lambda|\Psi_A - \Psi_B|^2 = 0$, where λ is a constant multiplier, than direct use of Eq. (C7) [6]. Applying Eq. (34) to this form and differentiating the resultant equation with respect to a^*_l and b^*_l, respectively, gives

$$\lambda\begin{pmatrix} \mathbf{K}_{z_0} & -\mathbf{K}_{z_0} \\ -\mathbf{K}_{z_0} & \mathbf{K}_{z_0} \end{pmatrix}\begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix} = 0, \tag{41}$$

where

$$K^{ll'}_{z_0} = e^{i2\pi(l-l')z_0/d}. \tag{42}$$

Thus Eq. (40) is completed by including this term:

$$\begin{pmatrix} \mathbf{D}^A & \\ & \mathbf{D}^B \end{pmatrix}\begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix} = \begin{pmatrix} \mathbf{H}^A & \\ & \mathbf{H}^B \end{pmatrix}\begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix} + \frac{1}{2}\begin{pmatrix} \mathbf{J}^A_{z_0} - \bar{\mathbf{J}}^A_{z_0} & -\mathbf{J}^B_{z_0} + \bar{\mathbf{J}}^A_{z_0} \\ \mathbf{J}^A_{z_0} - \bar{\mathbf{J}}^B_{z_0} & -\mathbf{J}^B_{z_0} + \bar{\mathbf{J}}^B_{z_0} \end{pmatrix}\begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix} + \lambda\begin{pmatrix} \mathbf{K}_{z_0} & -\mathbf{K}_{z_0} \\ -\mathbf{K}_{z_0} & \mathbf{K}_{z_0} \end{pmatrix}\begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix}. \tag{43}$$

This is the most general matrix equation for the variational determination of eigen values and vectors from the multi-band envelope-function equation.

Coefficients a_l and b_l, however, are not independent, because we expand envelope functions in materials A and B by the same kind of basis functions (plane waves) and these are related by the condition of Eq. (C7). As the plane waves form linearly independent basis set, this condition dictates $a_l = b_l$ [see Eq. (34)]. Applying this result to Eqs. (35) and (36), and then adding the resultant equations, we obtain

$$\mathcal{E}\sum_{l'} a_{l'}\int_{L_A+L_B} dz e^{-i2\pi(l-l')z/d} = \sum_{l'} a_{l'}\left[\int_{L_A} dz e^{-i2\pi lz/d} H_A e^{i2\pi l'z/d} + \int_{L_B} dz e^{-i2\pi lz/d} H_B e^{i2\pi l'z/d}\right]$$
$$+ \sum_{l'} a_{l'}\left[e^{-i2\pi lz/d} J^A_z e^{i2\pi l'z/d} - e^{-i2\pi lz/d} J^B_z e^{i2\pi l'z/d}\right]_{z=z_0}, \tag{44}$$

which can be written in the matrix form

$$\left(\mathbf{H}_A+\mathbf{H}_B\right)+\left(\mathbf{J}^A_{z_0}-\mathbf{J}^B_{z_0}\right)\mathbf{a}=\mathcal{E}\mathbf{a}. \tag{45}$$

It should be noted that all the matrices $\mathbf{H}$ and $\mathbf{J}$ in the above equation should be symmetric in the expansion indices l and l'; this requires a type of "symmetrization" for these matrices as, for instance, $\mathbf{H}_A=\frac{1}{2}(H^{ll'}_A+H^{l'l}_A)$.

There is an additional condition in the variational form of Eq. (33). A further analysis on this type of variational expression leads to taking only real part of the equation [see Eq. (A1.10) in Ref. 17] :

$$\mathrm{Re}\left(\sum_{ll'} a^*_l a_{l'}(H_{ll'}-\mathcal{E}D_{ll'})\right)=0. \tag{46}$$

If we look for only real values of $\mathcal{E}$, this condition with "Re" leads to "Hermitianization" for the matrices in the equation:

$$\left(\mathbf{H}+\mathbf{H}^\dagger\right)-\mathcal{E}\left(\mathbf{D}+\mathbf{D}^\dagger\right)\mathbf{a}=0. \tag{47}$$

Applying this result to the flux-continuity term in Eq. (45), a bit of manipulation gives

$$\mathbf{J}^A_{a/2}+\mathbf{J}^A_{-a/2}=i\frac{4\pi(l-l')}{d}H^{(2)}_A\sin[\pi(l-l')z/d]. \tag{48}$$

Here we used the fact that the two independent interfaces chosen at $z_0=\pm a/2$ have opposite normal direction to the interface planes as shown in Fig. 1; and we applied the "symmetrization" on l and l' as discussed above. As the flux above is not Hermitian, this term vanishes upon the "Hermitianization". The flux-continuity term on the material B side also vanishes by the same procedure. Thus the resultant variational equation becomes

$$\mathcal{E}\mathbf{a}=(\mathbf{H}_A+\mathbf{H}_B)a\equiv\left(\mathbf{H}^{total}_A+\mathbf{W}\right)\mathbf{a}, \tag{49}$$

where the Hermitian matrix $\mathbf{H}_A+\mathbf{H}_B$ is

$$\mathbf{H}_A+\mathbf{H}_B=\int_{L_A}dze^{-i2\pi lz/d}H_Ae^{i2\pi l'z/d}+\int_{L_B}dze^{-i2\pi lz/d}H_Be^{i2\pi l'z/d},$$

and

$$\mathbf{H}^{total}_A=\int_{L_A+L_B}dze^{-i2\pi lz/d}H_Ae^{i2\pi l'z/d},\ \mathbf{W}=\int_{L_B}dze^{-i2\pi lz/d}(H_B-H_A)e^{i2\pi l'z/d}. \tag{50}$$

We notice that the result is the same as Eq. (8) in the usual envelope-function approximation. The disappearance of current-continuity term can be accounted for that (1) we define a unique envelope function over the entire SL structure (we expand the envelope functions in both material regions by the same kind of basis set and the envelope-function continuity condition makes these identical) and (2) the BPD is transformed into an SL potential in layer B so that the current-continuity is implicitly satisfied. It should be also noted that the final result is somewhat different in form from the one reported previously [6] due to the disappearance of the current-continuity term.

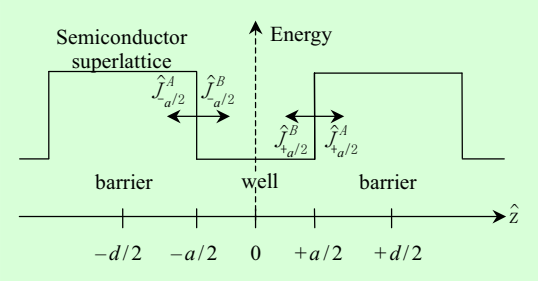

Fig. 1. Normal directions of current operators at SL interfaces.

For numerical computations, we take first an $In_{0.63}Ga_{0.37}As/In_{0.73}Ga_{0.27}As_{0.58}P_{0.42}$ SL with $60\,\mathring{A}/500\,\mathring{A}$ well/barrier widths and compare the results with those obtained by a transfer matrix method for a single quantum well with the same well width and material parameters [13]. As the model SL above has a long barrier width, the comparison in the first few confined

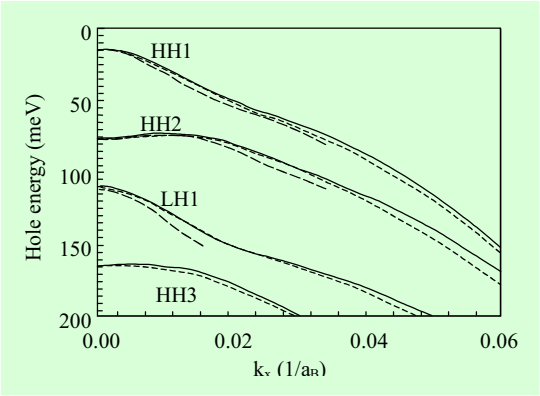

Fig. 2. The valence-band structure for $In_{0.63}Ga_{0.37}As/In_{0.73}Ga_{0.27}As_{0.58}P_{0.42}$ SL with $60\,\mathring{A}/500\,\mathring{A}$ well/barrier widths. The InGaAs layers are under compressive strain and InGaAsP layers are lattice matched to InP. The band-parameter difference is taken into account in the solid lines, while ignored in the dotted lines. The result for the single quantum well with the same well width by S. L. Chuang is displayed by the dashed lines. The barrier height is 180 meV.

subbands should be appropriate up to moderate k_t values of interest, because the SL subband widths are nearly zero for those bands. The envelope-function equation of Eq. (49) are solved variationally by expanding envelope functions in terms of 33 orthogonal sets, which are chosen as periodic plane waves $\exp(i2\pi lz/d)$, where l and d are an integer and the SL period, respectively [14]. Energies and envelope functions are obtained by numerical diagonalization of $(6\times33)\times(6\times33)$ matrix for each quantum state (k_x, n, q), where the three conduction, heavy-hole, and light-hole bands are included in the primary band group. Figure 2 shows that the two results are in a very close agreement

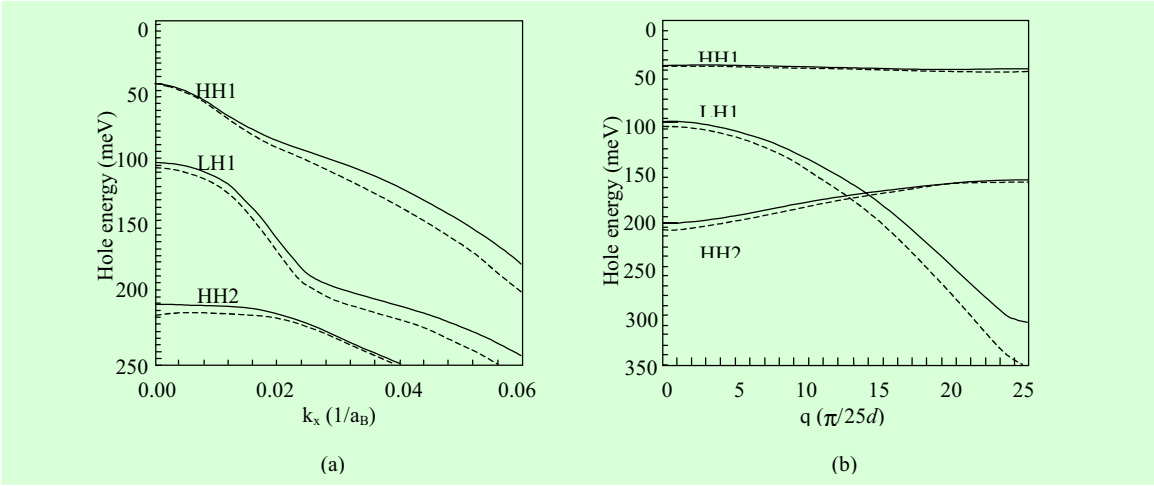

Fig. 3. The valence-band structure [(a) $\mathcal{E}-k_x$ and (b) $\mathcal{E}-q$ dispersions] for $In_{0.63}Ga_{0.37}As/In_{0.73}Ga_{0.27}As_{0.58}P_{0.42}$ SL with 30 Å/30 Å well/barrier widths. The band-parameter difference is taken into account in the solid lines, while ignored in the dotted lines. The barrier height is 180 meV.

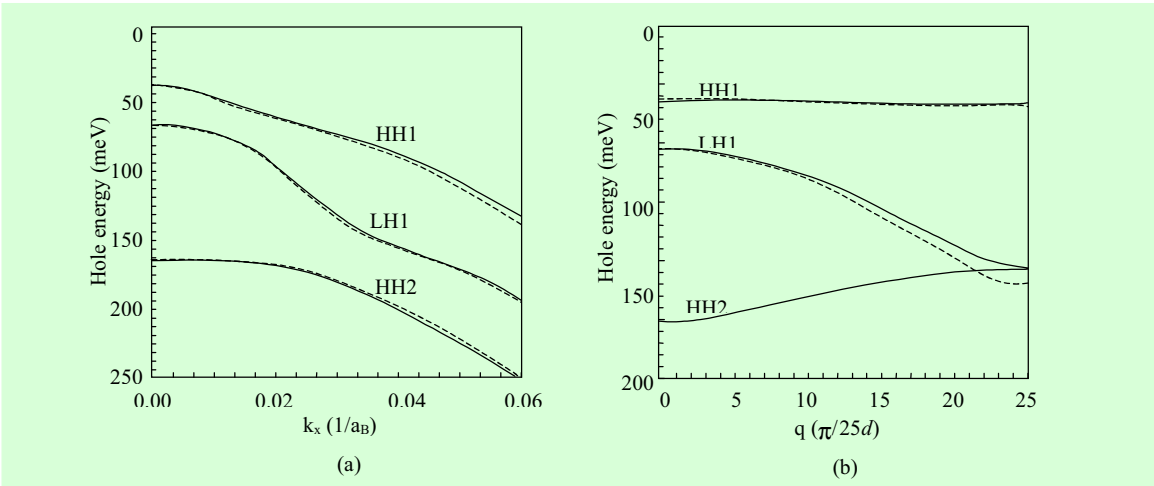

Fig. 4. The valence-band structure [(a) $\mathcal{E}-k_x$ and (b) $\mathcal{E}-q$ dispersions] for lattice-matched $GaAs/Al_{0.32}Ga_{0.68}As$ SL with 30 Å/30 Å well/barrier widths. The band-parameter difference is taken into account in the solid lines, while ignored in the dotted lines. The barrier height is 160 meV.

especially for HH1 and HH2 subbands; the agreement reduces for LH1 band as k_x increases, which may be due to errors mainly from using the axial approximation in the Chuang's calculation. The figure also shows that BPD does not considerably affect the overall energy structure for this SL structure.

Table 1. Band parameters. Values without designation are from Ref. [13], in which the notations used in the table are well described.

Parameters	GaAs	AlAs	InAs	InP	GaP	AlGaAs[a]	GaInAs[b]	GaInAsP[c]
a_0(Å)	5.6533	5.6600	6.0584	5.8688	5.4505	5.6554*	5.9085*	5.8688*
$\mathcal{E}_g$(eV)	1.42	3.03	0.36	1.35	2.74	1.82*	0.638	0.950
γ_1	6.85	3.45	20.4	4.95	4.05	6.03*	15.39*	11.71*
γ_2	2.1	0.68	8.3	1.65	0.49	1.79*	6.01*	4.41*
γ_3	2.9	1.29	9.1	2.35	1.25	2.45*	6.81*	5.18*
C_{11}^{d}	11.88	12.5	8.329	10.11	14.05	12.08*	9.642*	10.074*
C_{12}^{d}	5.38	5.34	4.526	5.61	6.203	5.37*	4.841*	5.180*
C_{44}^{d}	5.94	5.42	3.959	4.56	7.033	5.77*	4.692*	4.799*
a_v(eV)	−1.16	−2.47	−1.00	−1.27	−1.70	−1.58*	−1.06*	−1.19*
b(eV)	−1.7	−1.5	−1.8	−1.7	−1.8	−1.64*	−1.76*	−1.75*
d(eV)	−4.55	−3.4	−3.6	−5.6	−4.5	−4.18*	−3.95*	−4.46*

[a] $x = 0.32$ for $Al_xGa_{1-x}As$. [b] $x = 0.37$ for $Ga_xIn_{1-x}As$. [c] $x = 0.269$, $y = 0.581$ for $Ga_xIn_{1-x}As_yP_{1-y}$. [d] 10^{11}dyn/cm^2.
* Obtained by Linear interpolations.

Figure 3 shows the contribution of BPD to the subband energy structure for a 30 Å/30 Å InGaAs/InGaAsP SL. The material compositions are the same as before. As seen from the figures, in general, offsets in energy due to BPD becomes more noticeable for smaller well-barrier width SLs; and also become larger as k_t increases. This result can be expected because for smaller well-barrier width SLs, more particles spread into barrier layers, and this enhances the BPD effects.

We take another 30 Å/30 Å GaAs/$Al_{0.32}Ga_{0.68}As$ SL for a comparison. Figure 4 shows that BPD effect in this type of SL is much less than that of InGaAs/InGaAsP SL, as expected. The parameters used in the computations are summarized in Table 1. Band offsets of $Ga_xIn_{1-x}As/Ga_xIn_{1-x}As_yP_{1-y}$ SL were obtained by a transitivity between band-gap structures of the materials [13].

V. CONCLUSION

We presented a new description of envelope-function equation for SLs. The SL wave function and corresponding effective-mass equation have been formulated in terms of a linear combination of single basis set consisting of Bloch states for the constituent material with smaller band gap. Unlike most of previous treatments for the difference in the bulk Bloch functions as well as the band parameters between constituent materials, the present approach solves SL effective-mass equation as

a whole. In this description, these differences can be transformed into an SL potential in material layers with larger band gap. The symmetry of SL and the current-continuity at SL interfaces are implicitly taken into account through the order in perturbation theory at which the bulk Bloch function at $\mathbf{k}$ is obtained in terms of the zone-center Bloch functions. The present description is simplified significantly in the usual envelope-function approximation, and provides easier implementation of numerical computations because it does not require the interface matching, and, in many cases, band parameters are empirically known.

We reviewed the fundamental concepts of the motion of a wave packet and the velocity and acceleration theorems in the SL subjected to steady and uniform electric fields. We showed that the average of SL crystal momentums $\mathbf{K} = (k_x, k_y, q)$ included in a wave packet satisfies the equation of motion $\langle \mathbf{K} \rangle = \langle \mathbf{K} \rangle_0 + \mathbf{F}t/\hbar$, where $\mathbf{F}$ is the external electric field; and that the velocity and acceleration theorems provide the group velocity of the packet $\mathbf{v}_g = (1/\hbar)\nabla_{\mathbf{K}}\mathcal{E}(\mathbf{K})$ and definition of the effective mass tensor, respectively, in the SL structure. This review would provide a mathematical justification for the use of the fundamental concept of bulk effective-mass representation in SLs; i.e., the charge carriers in the additional SL periodic potential can still be treated as quasi particles described by the SL crystal momentum vectors K, and the standard formalisms in the effective-mass representation for bulk periodic solids, including $\mathbf{k}\cdot\mathbf{p}$ theory, are directly applicable to SL, as expected from its periodic structure.

We re-examined the variational procedure more thoroughly for solving the multiband SL envelope-function equation with inclusion of interface-matching conditions. The review was carried out based on the work of Schlosser and Marcus, and yielded variational equations in both general and reduced forms. We showed that, when envelope functions in different material layers are expanded by the same kind of basis functions, the current-continuity condition does not enter explicitly into the final equation; instead, the BPD acts as an SL potential in the larger band-gap material region. In this case, the variational equation becomes identical to the new description of SL equation presented in this paper in the usual envelope-function approximation. The variational equation turned out to be somewhat different from the one reported previously [6] in which the current-continuity term remains in the equation.

As an illustration of the application of the present work and also for a brief investigation of effects of BPD on the subband energy structure, we calculated by the proposed variational method energies non-strained of $GaAs/Al_{0.32}Ga_{0.68}As$ and $In_{0.63}\,Ga_{0.37}\,As/In_{0.73}\,Ga_{0.27}\,As_{0.58}\,P_{0.42}$ SLs strained with well/barrier widths of 60 Å / 500 Å and 30 Å / 30 Å. The result for the 60 Å / 500 Å InGaAs/InGaAsP SL showed a very close agreement with that obtained

with a transfer-matrix method by S. L. Chuang [13] for a single quantum well with the same well width and material parameters. It was also shown that the contribution of BPD to the energy structure becomes more noticeable for smaller well-barrier width SL structures. The result showed that BPD can be ignored for GaAs/AlGaAs SLs for large range of structural parameters; while ignoring BPD can cause appreciable errors for SLs such as InGaAs/InGaAsP SL especially with small well-barrier widths, as have been well established in the literature.

ACKNOWLEDGMENT

The authors wish to acknowledge Dr. K.C. Park, Mr. S.R. Kang, and Dr. C.H. Yim in ETRI for supporting this work.

APPENDIX A

The detailed algebraic steps for $H_{vv'}$ and $W_{vv'}$ of Eqs. (4) and (5) are as follows.

$$
\begin{aligned}
H_{vv'}(\mathbf{k},\mathbf{k}') &= \langle v,0|e^{-i\mathbf{k}\cdot\mathbf{r}}H_0^A + V^A|v',\mathbf{k}'\rangle_A \\
&\cong \mathcal{E}_{v,0}^A + \frac{\hbar^2k^2}{2m_0}\cdot\delta_{vv'}\delta_{\mathbf{k},\mathbf{k}'} + \frac{\hbar}{m_0}\langle v,0|e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}}\mathbf{k}\cdot\mathbf{p}|v',0\rangle_A \\
&\quad + \left(\frac{\hbar}{m_0}\right)^2 \sum_{N\neq J} \frac{\langle v,0|e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}}\mathbf{k}'\cdot\mathbf{p}|N,0\rangle_A \langle N,0|e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}}\mathbf{k}'\cdot\mathbf{p}|v',0\rangle_A}{\mathcal{E}_{v,0}^A - \mathcal{E}_{N,0}^A} \\
&\cong \left(\mathcal{E}_{v,0}^A + \frac{\hbar^2k^2}{2m_0}\right)\delta_{vv'}\delta_{\mathbf{k},\mathbf{k}'} + \frac{\hbar}{m_0}\langle v,0|\mathbf{k}\cdot\mathbf{p}|v',0\rangle_A\,\delta_{\mathbf{k},\mathbf{k}'} \\
&\quad + \left(\frac{\hbar}{m_0}\right)^2 \sum_{N\neq J} \frac{\langle v,0|\mathbf{k}'\cdot\mathbf{p}|N,0\rangle_A \langle N,0|\mathbf{k}'\cdot\mathbf{p}|v',0\rangle_A}{\mathcal{E}_{v,0}^A - \mathcal{E}_{N,0}^A}\delta_{\mathbf{k},\mathbf{k}'}, \qquad \text{(A1)}
\end{aligned}
$$

$$
\begin{aligned}
W_{vv'}(\mathbf{k},\mathbf{k}') &= \langle v,0|e^{-i\mathbf{k}\cdot\mathbf{r}}H_0^B + V^B|\theta_z^B|v',\mathbf{k}'\rangle_A - \langle v,0|e^{-i\mathbf{k}\cdot\mathbf{r}}H_0^A + V^A|\theta_z^B|v',\mathbf{k}'\rangle_A \\
&= \sum_{l,l',\mathbf{k}''} \langle v,0|l,0\rangle_B \langle l,0|e^{-i\mathbf{k}\cdot\mathbf{r}}H_0^B + V^B|\theta_z^B|l',\mathbf{k}''\rangle_B \langle l',\mathbf{k}''|v',\mathbf{k}'\rangle_A - \langle v,0|e^{-i\mathbf{k}\cdot\mathbf{r}}H_0^A + V^A|\theta_z^B|v',\mathbf{k}'\rangle_A \\
&\cong \sum_{l,l',\mathbf{k}''} \langle v,0|l,0\rangle_B \left(\mathcal{E}_{l',0}^B + \frac{\hbar}{m_0}\mathbf{k}''\cdot\mathbf{p} + \frac{\hbar^2k''^2}{2m_0}\right)\langle l,0|e^{i(\mathbf{k}''-\mathbf{k})\cdot\mathbf{r}}|\theta_z^B|l',0\rangle_B \langle l',\mathbf{k}''|v',\mathbf{k}'\rangle_A
\end{aligned}
$$

$$
\begin{aligned}
&+\left(\frac{\hbar}{m_0}\right)^2 \sum_{l,l',\mathbf{k}''} \sum_{N\neq l'} \frac{{}^B\langle l,0|e^{i(\mathbf{k}''-\mathbf{k})\cdot\mathbf{r}}\mathbf{k}''\cdot\mathbf{p}\theta_z^B|N,0\rangle^B\, {}^B\langle N,0|\mathbf{k}''\cdot\mathbf{p}|l',0\rangle^B\, {}^A\langle v,0|l,0\rangle^B\, {}^B\langle v',\mathbf{k}''|v',\mathbf{k}'\rangle^A}{\mathcal{E}^B_{l',0}-\mathcal{E}^B_{N,0}} \\
&-{}^A\langle v,0|e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}}\left(\mathcal{E}^A_{v,0}+\frac{\hbar}{m_0}\mathbf{k}'\cdot\mathbf{p}+\frac{\hbar^2k'^2}{2m_0}\right)\theta_z^B|v',0\rangle^A \\
&-\left(\frac{\hbar}{m_0}\right)^2 \sum_{N\neq l'} \frac{{}^A\langle v,0|e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}}\mathbf{k}'\cdot\mathbf{p}\theta_z^B|N,0\rangle^A\, {}^A\langle N,0|\mathbf{k}'\cdot\mathbf{p}|v',0\rangle^A}{\mathcal{E}^A_{v,0}-\mathcal{E}^A_{N,0}} \\
&\cong \int dz e^{i(k'_z-k_z)z}\Bigg\{\sum_l (c^l_{v'})^* c^l_v\left(\mathcal{E}^B_{l,0}+\frac{\hbar^2k'^2}{2m_0}-\mathcal{E}^A_{v,0}+\frac{\hbar^2k'^2}{2m_0}\right)\theta_z^B\delta_{\mathbf{k}_t,\mathbf{k}'_t} \\
&+\frac{\hbar}{m_0}\sum_{l,l'}(c^{l'}_{v'})^* c^l_v\, {}^B\langle l,0|\mathbf{k}'\cdot\mathbf{p}|l',0\rangle^B - {}^A\langle v,0|\mathbf{k}'\cdot\mathbf{p}|v',0\rangle^A\Big\}\theta_z^B\delta_{\mathbf{k}_t,\mathbf{k}'_t} \\
&+\left(\frac{\hbar}{m_0}\right)^2 \int dz e^{i(k'_z-k_z)z}\sum_{l,l'}\sum_{N\neq l'}(c^{l'}_{v'})^* c^l_v \frac{{}^B\langle l,0|\mathbf{k}'\cdot\mathbf{p}|N,0\rangle^B\, {}^B\langle N,0|\mathbf{k}'\cdot\mathbf{p}|l',0\rangle^B}{\mathcal{E}^B_{l',0}-\mathcal{E}^B_{N,0}}\theta_z^B\delta_{\mathbf{k}_t,\mathbf{k}'_t} \\
&-\left(\frac{\hbar}{m_0}\right)^2 \int dz e^{i(k'_z-k_z)z}\sum_{N\neq J}\frac{{}^A\langle v,0|\mathbf{k}'\cdot\mathbf{p}|N,0\rangle^A\, {}^A\langle N,0|\mathbf{k}'\cdot\mathbf{p}|v',0\rangle^A}{\mathcal{E}^A_{v,0}-\mathcal{E}^A_{N,0}}\theta_z^B\delta_{\mathbf{k}_t,\mathbf{k}'_{t'}}. \qquad \text{(A2)}
\end{aligned}
$$

In the above, we use approximations that (1) in the integrals above the fast (cell periodic Bloch functions) and slow (exponential functions) varying parts are integrated separately; (2) the domain of θ_z^B is assumed to be much longer than the size of the lattice, so that θ_z^B is taken out of the integration with fast varying part; finally, (3) ${}^B\langle l,\mathbf{k}'|v,\mathbf{k}\rangle^A \cong c^v_l\delta_{\mathbf{k},\mathbf{k}'}$. Introducing the description of Eq. (7) for the $\mathbf{k}\cdot\mathbf{p}$ perturbation terms, we obtain the results of Eqs. (4) and (5).

APPENDIX B

In this Appendix detailed algebraic steps taken to evaluate the velocity operator are presented.

$$
\begin{aligned}
&\frac{i}{\hbar}\,{}'\mathbf{k}_t,n,q|Hz-zH|\mathbf{k}'_t,n',q'\rangle \\
&=\frac{i}{\hbar}\mathcal{E}(\mathbf{k}_t,n,q)\,{}'\mathbf{k}_t,n,q|z|\mathbf{k}'_t,n',q'\rangle-\frac{i}{\hbar}\,{}'\mathbf{k}_t,n,q|z|\mathbf{k}'_t,n',q'\rangle\mathcal{E}(\mathbf{k}'_t,n',q') \\
&=\frac{1}{\hbar}\frac{\partial}{\partial q}\mathcal{E}(\mathbf{k}_t,n,q). \qquad \text{(B1)}
\end{aligned}
$$

Here

$$\langle \mathbf{k}_t, n, q|z|\mathbf{k}'_t, n', q'\rangle = \sum_{v,k_z}\sum_{v',k'_z} a(v,\mathbf{k}_t,n,q;k_z)^* \langle v,\mathbf{k}|z|v',\mathbf{k}'\rangle a(v',\mathbf{k}'_t,n',q';k'_z)$$
$$= \sum_{v,k_z} a(v,\mathbf{k}_t,n,q;k_z)^* i\frac{\partial}{\partial k_z} a(v,\mathbf{k}_t,n',q';k_z)\delta(\mathbf{k}'_t-\mathbf{k}_t)$$
$$+ \sum_{v,v',k_z} a(v,\mathbf{k}_t,n,q;k_z)^* F_{vv'} a(v',\mathbf{k}_t,n',q';k_z)\delta(\mathbf{k}'_t-\mathbf{k}_t), \tag{B2}$$

and

$$\langle v,\mathbf{k}|z|v',\mathbf{k}'\rangle = \int d^3r e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}} u_v^*(\mathbf{k},\mathbf{r}) z u_{v'}(\mathbf{k}',\mathbf{r})$$
$$= i\frac{\partial}{\partial k_z}\int d^3r e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}} u_v^*(\mathbf{k},\mathbf{r}) u_{v'}(\mathbf{k}',\mathbf{r}) - i\int d^3r e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}} \left(\frac{\partial}{\partial k_z} u_v^*(\mathbf{k},\mathbf{r})\right) u_{v'}(\mathbf{k}',\mathbf{r})$$
$$\equiv \delta_{vv'} i\frac{\partial}{\partial k_z}\delta(\mathbf{k}'-\mathbf{k}) + F_{vv'}\delta(\mathbf{k}'-\mathbf{k}), \tag{B3}$$

where

$$F_{vv'} = -i\frac{(2\pi)^3}{\Omega}\int d^3r \left(\frac{\partial}{\partial k_z} u_v^*(\mathbf{k},\mathbf{r})\right) u_{v'}(\mathbf{k},\mathbf{r}). \tag{B4}$$

The first term on the right hand side of Eq. (B2) can be simplified further to be

$$\sum_{v,k_z} a(v,\mathbf{k}_t,n,q;k_z)^* i\frac{\partial}{\partial k_z} a(v,\mathbf{k}_t,n',q';k_z)\delta(\mathbf{k}'_t-\mathbf{k}_t)$$
$$= \sum_{v,k_z}\left(\int \Psi^*(v,\mathbf{k}_t,n,q;z)e^{ik_z z}dz\right) i\frac{\partial}{\partial k_z}\left(\int \Psi(v,\mathbf{k}_t,n',q';z')e^{-ik_z z'}dz'\right)\delta(\mathbf{k}'_t-\mathbf{k}_t)$$
$$= \sum_{v,k_z}\int dz\Psi^*(v,\mathbf{k}_t,n,q;z) z \Psi(v,\mathbf{k}_t,n',q';z)\delta(\mathbf{k}'_t-\mathbf{k}_t)$$
$$= \sum_{v}\int dz\varphi^*(v,\mathbf{k}_t,n,q;z)e^{-iqz} z \varphi(v,\mathbf{k}_t,n',q';z)e^{iq'z}\delta(\mathbf{k}'_t-\mathbf{k}_t)$$
$$= i\frac{\partial}{\partial q}\delta(q-q')\delta(\mathbf{k}'_t-\mathbf{k}_t)\delta_{nn'} + \delta(q-q')\delta(\mathbf{k}'_t-\mathbf{k}_t)Y_{nn'}, \tag{B5}$$

The second term on the right hand side of Eq. (B2) can also be simplified to be

$$\sum_{v,v',k_z} a(v,\mathbf{k}_t,n,q;k_z)^* F_{vv'} a(v',\mathbf{k}_t,n',q';k_z)$$
$$= \sum_{v,v',k_z}\left(\int \Psi^*(v,\mathbf{k}_t,n,q;z)e^{ik_z z}dz\right)\left(F_{vv'}^{(0)} + k_z F_{vv'}^{(1)} + k_z F_{vv'}^{(2)} + \cdots\right)\left(\int \Psi(n',\mathbf{k}_t,n',q';z')e^{-ik_z z'}dz'\right)$$

$$
\begin{aligned}
&= \sum_{v,v'} F_{vv'}^{(0)} \int \Psi^*(v,\mathbf{k}_t,n,q;z)\Psi(v',\mathbf{k}_t,n',q';z)dz \\
&+ \sum_{v,v'} \int \Psi^*(v,\mathbf{k}_t,n,q;z)\Psi(v',\mathbf{k}_t,n',q';z') \left[F_{vv'}^{(1)} \frac{\partial}{\partial z}\delta(z-z') + F_{vv'}^{(2)} \frac{\partial^2}{\partial z^2}\delta(z-z') + \cdots \right] dzdz' \\
&= \sum_{v,v'} F_{vv'}^{(0)} \int e^{i(q'-q)z}\varphi^*(v,\mathbf{k}_t,n,q;z)\varphi(v',\mathbf{k}_t,n',q';z)dz \\
&\equiv \delta(q-q')X_{nn'}, \qquad \text{(B6)}
\end{aligned}
$$

where $F_{vv'}$ is expanded in the power of k_z:

$$
\begin{aligned}
F_{vv'} &\cong i\frac{(2\pi)^3}{\Omega} \int d^3r \left[u_{v,0}^*(\mathbf{r}) + \sum_{L\neq J} \frac{\hbar}{m_0} \frac{\langle u_{v,0}|\mathbf{k}\cdot\mathbf{p}|u_{L,0}\rangle}{\mathcal{E}_v^0 - \mathcal{E}_L^0} u_{L,0}^*(\mathbf{r}) + \cdots \right] \\
&\quad \times \frac{\partial}{\partial k_z} \left[u_{v',0}(\mathbf{r}) + \sum_{L'\neq J'} \frac{\hbar}{m_0} \frac{\langle u_{L',0}|\mathbf{k}\cdot\mathbf{p}|u_{v',0}\rangle}{\mathcal{E}_{v'}^0 - \mathcal{E}_{L'}^0} u_{L',0}(\mathbf{r}) + \cdots \right] \\
&\equiv F_{vv'}^{(0)} + k_z F_{vv'}^{(1)} + k_z^2 F_{vv'}^{(2)} + \cdots. \qquad \text{(B7)}
\end{aligned}
$$

Note that the higher order terms beyond $F_{vv'}^{(0)}$ vanish when they are included in the integration as above due to parity of the periodic part of SL envelope functions. Substituting the above results into Eq. (B2) gives

$$
\langle \mathbf{k}_t n, q|z|\mathbf{k}_t', n', q'\rangle = i\frac{\partial}{\partial q}\delta(q-q')\delta_{nn'} + \delta(q-q')(X_{nn'} + Y_{nn'}) \quad \delta(\mathbf{k}_t' - \mathbf{k}_t). \qquad \text{(B8)}
$$

APPENDIX C

The current operator in the envelope-function approximation has been studied by many researchers [4], [5], [10], [13]. Here, we briefly but rather explicitly review the derivation of the operator. The present description is closely related to the works by Smith [9] and Altarelli [6].

As the SL includes two different types of materials, local Hamiltonians in each material region can be defined as

$$
H^s = \frac{p^2}{2m} + V^S, \qquad \text{(C1)}
$$

where $s = A, B$. Corresponding Bloch states in each material can be written as

$$
\Psi_{\mathbf{k}}(r) = e^{i\mathbf{k}\cdot\mathbf{r}} \sum_d c_{d\mathbf{k}} u_{d\mathbf{k}}(r), \qquad \text{(C2)}
$$

where d is the band index in the primary group and bands not included in this group are distinguished by index β. The expansion coefficient $c_{d\mathbf{k}}$ are obtained by solving the eigenvalue equation of

$$[H_{dd'}(\mathbf{k}) - \mathcal{E}\delta_{dd'}]\, c_{d'\mathbf{k}} = 0, \tag{C3}$$

where $\mathcal{E}$ is the state energy and

$$H_{dd'}(\mathbf{k}) \equiv \langle u_d | e^{-i\mathbf{k}\cdot\mathbf{r}} H e^{i\mathbf{k}\cdot\mathbf{r}} | u_{d'\mathbf{k}} \rangle. \tag{C4}$$

Equation (C3) can be rewritten to display the k_z dependence of $H_{dd'}(\mathbf{k})$ explicitly as

$$\left[H^{(2)}_{dd'}(k_z)^2 + H^{(1)}_{dd'}(k_z) + H^{(0)}_{dd'} \right] c_{d'\mathbf{k}} = 0, \tag{C5}$$

where the matrices above are given by

$$\begin{aligned}
H^{(2)}_{dd'} &= \frac{\hbar^2}{2m}\delta_{dd'} + \left(\frac{\hbar}{m}\right)^2 \sum_{\beta} \frac{\langle u_d | p_z | u_\beta \rangle \langle u_\beta | p_z | u_{d'} \rangle}{(\mathcal{E}_d + \mathcal{E}_{d'})/2 - \mathcal{E}_\beta}, \\
H^{(1)}_{dd'} &= \frac{\hbar}{m} \langle u_d | p_z | u_{d'} \rangle + \left(\frac{\hbar}{m}\right)^2 \mathbf{k}_t \cdot \sum_{\beta} \left[\frac{\langle u_d | p_z | u_\beta \rangle \langle u_\beta | \mathbf{p}_t | u_{d'} \rangle}{(\mathcal{E}_d + \mathcal{E}_{d'})/2 - \mathcal{E}_\beta} + \frac{\langle u_d | \mathbf{p}_t | u_\beta \rangle \langle u_\beta | p_z | u_{d'} \rangle}{(\mathcal{E}_d + \mathcal{E}_{d'})/2 - \mathcal{E}_\beta} \right], \\
H^{(0)}_{dd'} &= \left[\mathcal{E}_d + \frac{\hbar^2 \mathbf{k}_t^2}{2m} - \mathcal{E} \right] \delta_{dd'} + \frac{\hbar \mathbf{k}_t}{m} \cdot \langle u_d | \mathbf{p}_t | u_{d'} \rangle + \frac{\hbar \mathbf{k}_t}{m} \cdot \sum_{\beta} \frac{\langle u_d | \mathbf{p}_t | u_\beta \rangle \langle u_\beta | \mathbf{p}_t | u_{d'} \rangle}{(\mathcal{E}_d + \mathcal{E}_{d'})/2 - \mathcal{E}_\beta} \cdot \frac{\hbar \mathbf{k}_t}{m}.
\end{aligned} \tag{C6}$$

In the above, the energy denominators for off-diagonal second-order matrix elements are symmetrized.

The boundary conditions for the envelope function can be obtained based on the reasonable assumption that the lattice-periodic basis functions are the same for both materials. On this assumption, the continuity condition for the total envelope function of Eq. (C2) implies continuity of the envelopes [6]

$$\Psi_{\mathbf{k}_t d}(z_0^-) = \Psi_{\mathbf{k}_t, d}(z_0^+) \tag{C7}$$

at interfaces z_0, where the continuity for each basis component results from the fact that the lattice-periodic basis functions are linearly independent. It is noted that the assumption made here corresponds to the approximation of $c_v^l = \delta_{v,l}$ in Sec. II.

The probability current is given by

$$\langle \Psi_{\mathbf{k}} | H - \mathcal{E} | \Psi_{\mathbf{k}} \rangle - \langle \Psi^*_{\mathbf{k}} | H - \mathcal{E} | \Psi^*_{\mathbf{k}} \rangle = \frac{\hbar^2}{2im} \int_S dS\hat{n} \cdot (\Psi^*_{\mathbf{k}} \nabla \Psi_{\mathbf{k}} - \Psi_{\mathbf{k}} \nabla \Psi^*_{\mathbf{k}}), \tag{C8}$$

Table 2a. Matrix $H^{(2)}$.

	c1	c2	h1	h2	l1	l2
c1	$-\gamma_c$					
c2		$-\gamma_c$				
h1			$\tilde{\gamma}^-$			
h2				$\tilde{\gamma}^-$		
l1					$\tilde{\gamma}^+$	
l2						$\tilde{\gamma}^+$

Table 2b. Matrix $H^{(1)}$.

	c1	c2	h1	h2	l1	l2
c1					$-\sqrt{2/3}P_0$	
c2						$-i\sqrt{2/3}P_0$
h1					$-i2\sqrt{3}\gamma_3 k_t^+$	
h2						$i2\sqrt{3}\gamma_3 k_t^-$
l1	$\sqrt{2/3}P_0$		$-i2\sqrt{3}\gamma_3 k_t^-$			
l2		$-i\sqrt{2/3}P_0$		$i2\sqrt{3}\gamma_3 k_t^+$		

where S is the surface of the interface and $\hat{n}$ is a unit outward normal to S. In our case, as the probability current in the z-direction must be the same across all planes perpendicular to $\hat{z}$, it can be averaged over a unit SL cell to give

$$\langle \Psi_{\mathbf{k}} | H - \mathcal{E} | \Psi_{\mathbf{k}} \rangle - \langle \Psi_{\mathbf{k}}^* | H - \mathcal{E} | \Psi_{\mathbf{k}}^* \rangle = i\hbar S \hat{z} \cdot \langle \Psi_{\mathbf{k}} | j_z(z) | \Psi_{\mathbf{k}} \rangle_{avg}, \tag{C9}$$

where

$$\langle \Psi_{\mathbf{k}} | j_z(z) | \Psi_{\mathbf{k}} \rangle_{avg} \equiv \frac{\hbar}{2im} \left[\langle \Psi_{\mathbf{k}} | \partial_z | \Psi_{\mathbf{k}} \rangle - \langle \Psi_{\mathbf{k}}^* | \partial_z | \Psi_{\mathbf{k}}^* \rangle \right]. \tag{C10}$$

Substituting Eq. (C2) into Eq. (C10) gives

$$\begin{aligned}
&\langle \Psi_{\mathbf{k}} | j_z(z) | \Psi_{\mathbf{k}} \rangle_{avg} \\
&= 2 \left\{ \sum_{dd'} \left\{ \frac{\hbar}{2m} \delta_{dd'} + \left(\frac{\hbar}{m} \right)^2 \sum_{\beta} \frac{\langle u_d | p_z | u_\beta \rangle \langle u_\beta | p_z | u_{d'} \rangle}{(\mathcal{E}_d + \mathcal{E}_{d'})/2 - \mathcal{E}_\beta} \right\} k_z \right. \\
&\quad \left. + \sum_{dd'} \left\{ \frac{\hbar}{m} \right\} \langle u_d | p_z | u_{d'} \rangle + \left(\frac{\hbar}{m} \right)^2 \sum_{\beta} \frac{\langle u_d | \mathbf{k}_t \cdot \mathbf{p}_t | u_\beta \rangle \langle u_\beta | p_z | u_{d'} \rangle}{(\mathcal{E}_d + \mathcal{E}_{d'})/2 - \mathcal{E}_\beta} + \left(\frac{\hbar}{m} \right)^2 \sum_{\beta} \frac{\langle u_d | p_z | u_\beta \rangle \langle u_\beta | \mathbf{k}_t \cdot \mathbf{p}_t | u_{d'} \rangle}{(\mathcal{E}_d + \mathcal{E}_{d'})/2 - \mathcal{E}_\beta} \right\} \\
&= \sum_{dd'} \left\{ 2H^{(2)}_{dd'} k_z + H^{(1)}_{dd'} \right\},
\end{aligned} \tag{C11}$$

where we use

$$\langle u_\beta | \mathbf{k} \cdot \mathbf{p} | u_d \rangle^* = \langle u_d | \mathbf{k} \cdot \mathbf{p} | u_\beta \rangle \quad \text{and} \quad \langle u_{d'}^* | p_z | u_d^* \rangle = - \langle u_d | p_z | u_{d'} \rangle. \tag{C12}$$

Translation of Eq. (C11) into the current operator for the envelope functions can be made by replacing $k_z \rightarrow -i\partial_z$:

$$J_z^{dd'} = -2iH^{(2)}_{dd'} \partial_z + H^{(1)}_{dd'}. \tag{C13}$$

The matrices $H^{(2)}_{dd'}$ and $H^{(1)}_{dd'}$ are given in Tables 2a and 2b for a 6×6 envelope-function equation. Note that $H^{(2)}_{dd'}$ is Hermitian but $H^{(1)}_{dd'}$ not Hermitian. The basis functions for these tables are chosen as

$$
\begin{aligned}
c1(\Gamma_6,1/2) &= |s\uparrow\rangle,\\
c2(\Gamma_6,-1/2) &= |s\downarrow\rangle,\\
h1(\Gamma_8,3/2) &= \frac{1}{\sqrt{2}}|(X+iY)\uparrow\rangle,\\
h2(\Gamma_8,-3/2) &= \frac{1}{\sqrt{2}}|(iX+Y)\downarrow\rangle,\\
l1(\Gamma_8,1/2) &= \frac{1}{\sqrt{6}}|(iX-Y)\downarrow\rangle - i\frac{\sqrt{2}}{\sqrt{3}}|Z\uparrow\rangle,\\
l2(\Gamma_8,-1/2) &= \frac{1}{\sqrt{6}}|(X-iY)\uparrow\rangle + \frac{\sqrt{2}}{\sqrt{3}}|Z\downarrow\rangle,
\end{aligned}
\tag{C14}
$$

where the label Γ specifies the irreducible representation of the T_d double group; $|s\rangle$ represents the s-like spatial function, and $|x\rangle$, $|y\rangle$, and $|z\rangle$ represent the p-like functions; and the arrows designate the two eigenspinors of the operator σ_z:

$$
\uparrow = \begin{bmatrix}1\\0\end{bmatrix} \text{ and } \downarrow = \begin{bmatrix}0\\1\end{bmatrix}. \tag{C15}
$$

The quantities included in the tables are defined as

$$
\begin{aligned}
&\gamma^{\pm} = \gamma_1 \pm \gamma_2,\ \bar{\gamma}^{\pm} = \gamma_1 \pm 2\gamma_2,\\
&P_0 = -i\frac{\hbar}{m_0}\langle s|p_x|\Gamma_4 j\rangle,\\
&k_t^{\pm} = k_x \pm ik_y,\ \gamma_c = A' + 1,
\end{aligned}
\tag{C16}
$$

and [18]

$$
A' = \frac{\hbar^2}{m_0^2}\sum_{nj}\frac{\langle s|p_x|n\Gamma_4 j\rangle^2}{\mathcal{E}-\mathcal{E}_{n\Gamma_4}}, \tag{C17}
$$

where j labels the row to which the function associated with Γ belongs, and n specifies the band (in the summation the bottom of conduction band with energy of $\mathcal{E}_c$ is not included because this band is included in the primary band set).

The modified Luttinger parameters above are related to the original Luttinger parameters with superscript L by [19]

$$
\begin{aligned}
&\gamma_1 = \gamma_1^L - \frac{\mathcal{E}_P}{3\mathcal{E}_g+\Delta},\ \gamma_2 = \gamma_2^L - \frac{1}{2}\frac{\mathcal{E}_p}{3\mathcal{E}_g+\Delta},\\
&\text{and } \gamma_3 = \gamma_3^L - \frac{1}{2}\frac{\mathcal{E}_p}{3\mathcal{E}_g+\Delta},
\end{aligned}
\tag{C18}
$$

where $\mathcal{E}_g$ is the band gap between the conduction band (Γ_6) and the valence band (Γ_8), and

$$
\mathcal{E}_p = \frac{2m_0}{\hbar^2}p_0^2. \tag{C19}
$$

The current-continuity condition for the envelope functions is obtained by operating Eq. (C13) on the envelopes at the interfaces:

$$
\begin{aligned}
&\sum_{v'} J_z^{vv'}(z_0^-)\Psi_{\mathbf{k}_t,v'}(z_0^-)\\
&= \sum_{v'} J_z^{vv'}(z_0^+)\Psi_{\mathbf{k}_t,v'}(z_0^+).
\end{aligned}
\tag{C20}
$$

Equations (C7) and (C20) establish the necessary boundary conditions for the envelope functions across the interfaces.

REFERENCES

[1] L. Esaki and R. Tsu, "Superlattice and Negative Differential Conductivity in Semiconduc-

tors," *IBM J. Res. Develop.*, Vol. 14, 1970, pp. 61−65.

[2] P.A. Lebwohl and R. Tsu, "Electrical Transport Properties in a Superlattice," *J. Appl. Phys.*, Vol. 41, No. 6, 1970, pp. 2664−2667.

[3] R.F. Kazarinov and R.A. Suris, "Electrical and Electromagnetic Properties of Semiconductors with a Superlattice," *Soviet Phys. Semicon.*, Vol. 6, No. 1, 1972, pp. 120−131.

[4] S.R. White and L.J. Sham, "Electronic Properties of Flat-Band Semiconductor Heterostructures," *Phys. Rev. Lett.*, Vol. 47, No. 12, 1981, pp. 879−882.

[5] G. Bastard, "Superlattice Band Structure in the Envelope-Function Approximation," *Phys. Rev. B*, Vol. 24, No. 10, 1981, pp. 5693−5697; *ibid.* "Theoretical Investigations of Superlattice Band Structure in the Envelope-Function Approximation," Vol. 25, No. 12, 1982, pp. 7584−7596; G. Bastard and J.A. Brum, "Electronic States in Semiconductor Heterostructures," *IEEE Journal of Quantum Electronics*, Vol. QE-22, No. 9, 1986, pp. 1625−1644.

[6] M. Altarelli, "Application of High Magnetic Fields in Semiconductor Physics," Proceedings, Grenoble, France, 174 (1982), in Edited by G. Landwehr; M. Altarelli, "Electronic Structure and Semiconductor-Semimetal Transition in InAs-GaSb Superlattice," *Phys. Rev.* B, Vol. 28, No. 2, 1983, pp. 842−845; M. Altarelli and U. Ekenberg, "Calculations of Hole Subbands in Semiconductor Quantum Wells and Superlattices," *Phys. Rev.* B, Vol. 32, No. 8, 1985, pp. 5138−5143.

[7] D.A. Broido and L.J. Sham, "Effective Masses of Holes at GaAs-AlGaAs Heterojunctions," *Phys. Rev. B*, Vol. 31, No. 2, 1985, pp. 888−892.

[8] W. Pötz, W. Porod, and D.K. Ferry, "Theoretical Study of Subband Levels in Semiconductor Heterostructures," *Phys. Rev.* B, Vol. 32, No. 6, 1985, pp. 3868−3875.

[9] D.L. Smith and C. Mailhiot, "**k**·**p** Theory of Semiconductor Superlattice Electronic Structure. I. Formal Results," *Phys. Rev. B*, Vol. 33, No. 12, 1986, pp. 8345−8359; C. Mailhiot and D.L. Smith, "**k**·**p** Theory of Semiconductor Superlattice Electronic Structure. II. Application to $Ga_{1-x}In_xAs$-$Al_{1-y}In_yAs$," *Phys. Rev. B*, Vol. 33, No. 12, 1986, pp. 8360−8372.

[10] L.C. Andreani, A. Pasquarello, and F. Bassani, "Hole Subbands in Strained GaAs-$Ga_{1-x}Al_xAs$ Quantum Wells: Exact Solution of the Effective-Mass Equation," *Phys. Rev. B*, Vol. 36, No. 11, 1987, pp. 5887−5894.

[11] N.F. Johnson, H. Ehrenreich, P.M. Hui, and P.M. Young, "Electronic and Optical Properties of III-V and II-VI Semiconductor Superlattices," *Phys. Rev. B*, Vol. 41, No. 6, 1990, pp. 3655−3669.

[12] Y.C. Chang and D.E. Aspens, *Phys. Rev. B*, Vol. 41, 1990, pp. 12002.

[13] S.L. Chuang, "Efficient Band-Structure Calculations of Strained Quantum Wells," *Phys. Rev. B*, Vol. 43, No. 12, 1991, pp. 9649−9661; *Physics of Optoelectronic Devices*, John Wiley & Sons, Inc., 1995.

[14] B.W. Kim and A. Majerfeld, "Electronic and Intersubband Optical Properties of p-type GaAs/AlGaAs Superlattices for Infrared Photodetectors," *J. Appl. Phys.*, Vol. 77, No. 9, 1995, pp. 4552−4558; B.W. Kim, E. Mao, and A. Majerfeld, "Analysis of Optical Properties of p-Type GaAs/AlGaAs Superlattices for Multi-wavelength Normal Incidence Photodetectors," J. *Appl. Phys.*, Vol. 81, No. 4, 1997, pp. 1883−1889.

[15] P.O. Lowdin, "A Note on the Quantum-Mechanical Perturbation Theory," *J. Chem. Phys.*, Vol. 19, No. 11, 1951, pp. 1396−1410.

[16] B.W. Kim Y.I. Jun, and H.B. Jung, "Improved Multi-band Transfer Matrix Method for Calculating Eigenvalues and Eigenfunctions of Quantum Well and Superlattice Structures," *ETRI Journal*, Vol. 20, No. 4, Dec. 1998, pp. 361−379.

[17] H. Schlosser and P.M. Marcus, "Composite Wave Variational Method for Solution of the Energy-Band Problem in Solids," *Phys. Rev.*, Vol. 131, No. 6, 1963, pp. 2529−2546.

[18] E.O. Kane, *Physics of III-V Compounds*, Vol. 1, edited by R.K. Willardson and A.C. Beer, Academic, New York, 1966, p. 75.

[19] J.M. Luttinger, "Quantum Theory of Cyclotron Resonance in Semiconductors: General Theory," *Phys. Rev.*, Vol. 102, No. 4, 1956, pp. 1030−1041.

[20] J. Callaway, *Quantum Theory of the Solid State*, Academic, New York, 1974, p. 466.

Byoung-Whi Kim received the Ph. D. degree in electrical and computer engineering from University of Colorado, Boulder, Colorado in 1993. From 1983 to 1988, he was involved in the development of a digital switching system in ETRI. Since he joined ETRI again in 1994, he has been working on III-V compound-semiconductor optical switches based on strain-induced piezoelectric effects. His research interests include theoretical physics of compound semiconductor materials and optoelectronic devices.

Yong Il Jun received the B.S. in electrical engineering from Korea University in 1981 and the M.S. in electrical engineering in KAIST in 1983. From 1983 to 1987, He was a researcher at Gold Star Precision and developed a front-end X-band receiver, and an antenna of direction finder. Since 1987, he has been a senior engineer of ETRI, and develops MMIC, U-interface PHY-layer protocol engine, and ATM switching chipsets. His current research areas are switching element, switching fabric, traffic control, and signal integrity of large-scale system.

Hee Bum Jung received the B.S. degree in electronics engineering from Sogang University, Seoul, Korea in 1981, the M.S. degree in electrical engineering from Korea Advanced Institute of Science and Technology in 1983, and the Ph.D. degree in electrical engineering from Columbia University, New York, New York, U.S.A. in 1992. From 1983 to 1987 he was with KIET (former ETRI), Gumi, Korea, where he was involved in the development of custom integrated circuit design and modeling. While in Columbia University, he was also a student intern (1990 to 1991) of AT&T Bell Laboratory, Murray Hill, NJ, U.S.A. with research topic of HBT modeling. He rejoined ETRI in 1993 to pursue VLSI circuit design. His interests include analog-digital mixed signal VLSI design, circuit modeling, and CMOS RF & analog front-end IC's for IMT-2000 terminal equipments.