Operator ordering in effective-mass theory for heterostructures. II. Strained systems

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A new kinetic-energy operator $-\frac{1}{2}\hbar^2 m^{\alpha} a^{\delta} \nabla m^{\beta} a^{-2\delta} \nabla m^{\alpha} a^{\delta}$ suitable for effective-mass treatment of strained heterostructures is introduced. Here, $m(\mathbf{r})$ is the local effective mass and $a(\mathbf{r})$ is the local lattice constant. By comparison of exact results with effective-mass results for solvable test models, values of α, β, and δ, which ensure asymptotic agreement, are determined. Based on qualitative similarities between the test models considered and realistic systems, the boundary conditions [$(1/a)\phi$=continuous], [$(a/m)\phi'$=continuous] are proposed for *abrupt* heterointerfaces for conduction-band states in strained systems. When a single-band effective-mass equation is applicable to hole states, however, we propose that the continuity of ϕ and $(1/m)\phi'$ should be imposed instead.

I. INTRODUCTION

In the preceding paper,[1] the problem of operator ordering in effective-mass theory for semiconductor heterostructures was addressed. The approach was to compare *exact* results for solvable test cases with the corresponding results from different candidates of effective-mass equations in order to sort out the right candidate, if any. The one-parameter family of kinetic-energy operators considered was

$$H_{\text{kin}} = \tfrac{1}{2} m^{\alpha} \mathbf{p} m^{\beta} \mathbf{p} m^{\alpha} , \tag{1}$$

where $m(\mathbf{r})$ is, in general, a position-dependent effective mass. It is a one-parameter family since $2\alpha+\beta=-1$. The operator (1) fulfills by construction the basic requirement of hermiticity. Binary heterostructures with *abrupt* interfaces were chosen as test models, and for analytic convenience the component materials were modeled as one-dimensional Kronig-Penney lattices. Closed-form conditions, both for extended miniband states in superlattices and for bound states in quantum wells and in local potentials at heterointerfaces, were obtained exactly and compared with the corresponding conditions found from effective-mass theory. It was demonstrated that asymptotic agreement between effective-mass results and exact results can only be achieved with $\alpha=0$ and $\beta=-1$. For heterostructures involving materials with *equal* lattice constants, asymptotic agreement for, e.g., the lowest subband edge and the quantum-well ground-state energy was explicitly shown in the limit of zero band offset between the two materials. For *unequal* lattice constants, however, no such asymptotic agreement existed in the general case. In many practical applications the condition of equality of lattice constants is well fulfilled. However, strained heterostructures have recently attracted much attention because of possible applications and interesting physics.[2] An effective-mass description that takes into account effects of spatially dependent lattice constants is thus called for. Also, as a matter of principle, the absence of asymptotic agreement is unsatisfactory and makes one wonder whether this could be cured by an alternative effective-mass treatment.

In this paper a natural generalization of the kinetic-energy operator (1) is proposed to deal with strained heterostructures, viz.,

$$H_{\text{kin}} = \tfrac{1}{2} m^{\alpha} a^{\delta} \mathbf{p} m^{\beta} a^{-2\delta} \mathbf{p} m^{\alpha} a^{\delta} . \tag{2}$$

It is Hermitian by construction and reduces to the operator (1) when the lattice constant a is the same throughout the heterostructure. However, for a spatially varying lattice constant $a(\mathbf{r})$ the effect of the additional factors will be felt. With the operator (2), the new effective-mass equation describing states close to a conduction-band edge, say, has the form

$$-\tfrac{1}{2}\hbar^2 m^{\alpha} a^{\delta} \nabla m^{\beta} a^{-2\delta} \nabla m^{\alpha} a^{\delta} \phi = [E - E^c(\mathbf{r}) - U(\mathbf{r})]\phi . \tag{3}$$

Here, $E^c(\mathbf{r})$ is the position-dependent conduction-band edge, and $U(\mathbf{r})$ is a possible extrinsic potential (for example due to impurities).

In order for the left-hand side of (3) to have, for heterostructures with abrupt interfaces, no stronger singularities than the right-hand side, the boundary conditions

$$m^{\alpha} a^{\delta} \phi = \text{continuous}; \quad m^{\alpha+\beta} a^{-\delta} \phi' = \text{continuous} \tag{4}$$

must be satisfied at heterointerfaces. To determine α, β, and δ we use the same strategy as in Ref. 1 and compare exact results for solvable test cases (with *abrupt* heterointerfaces) with effective-mass results obtained via the new boundary conditions (4). It will be demonstrated that asymptotic agreement in the zero-offset limit only can be achieved with

$$\alpha=0, \ \beta=-1, \ \delta=0 \text{ or } -1 . \tag{5}$$

The appropriate value of δ (0 or -1) depends on the properties of the conduction-band edges in question.

The rest of the paper is organized as follows. In Sec. II we consider models for superlattices, quantum wells, and

local potentials at heterointerfaces and show how the parameter values (5) are determined. In Sec. III, a handwaving argument, which makes the conclusions reached in Sec. II plausible, is presented. The application to realistic strained heterostructures is discussed in Sec. IV. A short summary is given in Sec. V.

II. DETERMINATION OF BOUNDARY-CONDITION PARAMETERS

In this section the form of the boundary conditions will, for solvable test cases, be determined by comparison between exact results and results from effective-mass theory. For definiteness and analytic convenience we only consider states energetically close to conduction-band edges. The exact solutions are identical to the ones in Ref. 1, while the effective-mass solutions are only slightly altered due to the new and more general boundary conditions (4). Details in the mathematical derivations will therefore be omitted in the presentation given below.

A. Superlattices

The superlattice is modeled as alternating layers of different Kronig-Penney materials. The layer widths of the layers are p_1a_1 and p_2a_2 for material 1 and 2, respectively, where p_1,p_2 are integers and a_1,a_2 are lattice constants. The Schrödinger equation to solve is

$$-\frac{\hbar^2}{2m_0}\frac{d^2\psi}{dx^2}+V(x)\psi=E\psi\ , \tag{6}$$

where

$$V(x)=\begin{cases} V_1-\dfrac{\hbar^2\alpha_1}{m_0a_1}\displaystyle\sum_{n=1}^{p_1}\delta(x-(n-\tfrac{1}{2})a_1) \\ \qquad\qquad \text{for } 0\le x<p_1a_1, \\ V_2-\dfrac{\hbar^2\alpha_2}{m_0a_2}\displaystyle\sum_{n=1}^{p_2}\delta(x-(n-\tfrac{1}{2})a_2-p_1a_1) \\ \qquad\qquad \text{for } p_1a_1\le x\le p_1a_1+p_2a_2, \end{cases} \tag{7}$$

and

$$V(x+p_1a_1+p_2a_2)=V(x)\ . \tag{8}$$

α_1 and α_2 are dimensionless strength parameters, and m_0 is the free-electron mass. In between the δ-function wells in material 1 (2) the potential is set to the constant value V_1 (V_2). The solution of (6)–(8) proceeds by standard transfer-matrix technique. Minibands exist for energies that satisfy the condition (Ref. 1)

$$\left|2\cos(p_1u_1)\cos(p_2u_2)-\eta_1\eta_2\sin(p_1u_1)\sin(p_2u_2)\left[\frac{a_2b_2\sin u_1}{a_1b_1\sin u_2}+\frac{a_1b_1\sin u_2}{a_2b_2\sin u_1}\right]\right|\le 2\ , \tag{9}$$

where we have defined the auxiliary variables q_i, u_i, b_i, and η_i as follows:

$$\frac{\hbar^2}{2m_0a_i^2}q_i^2=E-V_i\ , \tag{10}$$

$$\cos u_i=|\cos q_i-\alpha_i q_i^{-1}\sin q_i|,\quad 0\le u_i\le\pi/2 \tag{11}$$

$$b_i=q_i^{-1}\sin q_i-\alpha_i q_i^{-2}+\alpha_i q_i^{-2}\cos q_i\ , \tag{12}$$

and

$$\eta_i=\mathrm{sgn}(\cos q_i-\alpha_i q_i^{-1}\sin q_i)=\pm 1\ . \tag{13}$$

The definition of u_i (11) is only appropriate for energies that correspond to a *band* in pure bulk material i. Minibands may also occur for energies that correspond to a *gap* in one of the materials (the barrier material), however, and then the auxiliary variable v_i, defined via

$$\cosh v_i=|\cos q_i-\alpha_i q_i^{-1}\sin q_i|,\quad v_i\ge 0 \tag{14}$$

is used instead. Condition (9) still holds under the replacement $u_i\to -iv_i$. For notational simplicity we stick to the u variables in the discussion of superlattices below.

For superlattice states energetically close to the conduction-band edges of the constituent materials, the effective-mass equation to solve is

$$-\tfrac{1}{2}\hbar^2 m^{\alpha}a^{\delta}\frac{d}{dx}m^{\beta}a^{-2\delta}\frac{d}{dx}m^{\alpha}a^{\delta}\phi=[E-E^c(x)]\phi\ . \tag{15}$$

Once more the transfer-matrix technique is used, and the condition for minibands, analogous to the exact condition (9), is

$$\left|2\cos(p_1\bar{q}_1)\cos(p_2\bar{q}_2)-\sin(p_1\bar{q}_1)\sin(p_2\bar{q}_2)\left[\frac{a_2^{2\delta+1}m_1^{\beta}\bar{q}_1}{a_1^{2\delta+1}m_2^{\beta}\bar{q}_2}+\frac{a_1^{2\delta+1}m_2^{\beta}\bar{q}_2}{a_2^{2\delta+1}m_1^{\beta}\bar{q}_1}\right]\right|\le 2\ . \tag{16}$$

Here,

$$\frac{\hbar^2}{2m_ia_i^2}\bar{q}_i^{\,2}=E-E_i^c\ . \tag{17}$$

With $\delta=0$, condition (16) reduces to the effective-mass condition obtained in Ref. 1.

The question now arises whether there exist situations in which the approximate effective-mass condition (16) is in close agreement with the exact condition (9). In Ref. 1 it was shown that *near a band edge* u_i will be asymptotically equal to $\bar{q}_i$ (i.e., the same function of the energy E).

In Kronig-Penney lattices conduction-band edges occur for

$$q_{i,n}^{c}=n\pi, \quad n=1,2,3,\ldots \tag{18}$$

which corresponds to the energies

$$E_{i,n}^{c}=V_i+\frac{\hbar^2 n^2\pi^2}{2m_0 a_i^2} . \tag{19}$$

At these conduction-band edges one finds the effective masses

$$m_{i,n}=m_0\frac{\alpha_i}{n^2\pi^2}, \quad n=1,2,3,\ldots . \tag{20}$$

For energies close to the conduction-band edges the parameter b_i, defined in (12), is, to lowest nonvanishing order in u_i,

$$b_i=\begin{cases} -2\dfrac{m_i}{m_0}, & n \text{ odd} \\ \dfrac{m_0}{2\pi^2 n^2 m_i}u_i^2, & n \text{ even.} \end{cases} \tag{21}$$

When the two conduction-band edges in question are of the same type, i.e., have same band index n, condition (9) reduces to the asymptotic form

$$\left|2\cos(p_1u_1)\cos(p_2u_2)-\sin(p_1u_1)\sin(p_2u_2)\left[\frac{a_2}{a_1}\frac{m_2}{m_1}\frac{u_1}{u_2}+\frac{a_1}{a_2}\frac{m_1}{m_2}\frac{u_2}{u_1}\right]\right|\leq 2 \tag{22}$$

for *odd n*, and to

$$\left|2\cos(p_1u_1)\cos(p_2u_2)-\sin(p_1u_1)\sin(p_2u_2)\left[\frac{a_1}{a_2}\frac{m_2}{m_1}\frac{u_1}{u_2}+\frac{a_2}{a_1}\frac{m_1}{m_2}\frac{u_2}{u_1}\right]\right|\leq 2 \tag{23}$$

for *even n*. These conditions are to be compared with the effective-mass condition (16). For *odd-n* bands asymptotic agreement can only be achieved with

$$\beta=-1 \text{ and } \delta=0 , \tag{24}$$

while for *even-n* bands,

$$\beta=-1 \text{ and } \delta=-1 \tag{25}$$

is required. It should be stressed that in order for conditions (22) and (23) to be valid, the energy in question must be close to the conduction-band edges of *both* materials. This can only be fulfilled if the band offset

$$V_{\text{off}}=E_2^c-E_1^c \tag{26}$$

is small.

B. Quantum wells

A quantum well can be considered as the limiting case of a superlattice with increasing barrier width and thus does not represent an independent test. We choose material 2 to be the barrier material and take the $p_2\rightarrow\infty$ limit. The condition for a bound state is[1]

$$2\eta_1\eta_2\cot(p_1u_1)=\frac{a_2}{a_1}\frac{b_2}{b_1}\frac{\sin u_1}{\sinh v_2}-\frac{a_1}{a_2}\frac{b_1}{b_2}\frac{\sinh v_2}{\sin u_1} . \tag{27}$$

The effective-mass condition is obtained analogously as

$$2\cot(p_1\bar{q}_1)=\frac{a_2^{2\delta+1}}{a_1^{2\delta+1}}\frac{m_1^{\beta}}{m_2^{\beta}}\frac{\bar{q}_1}{\tilde{q}_2}-\frac{a_1^{2\delta+1}}{a_2^{2\delta+1}}\frac{m_2^{\beta}}{m_1^{\beta}}\frac{\tilde{q}_2}{\bar{q}_1} , \tag{28}$$

where $\tilde{q}_2$ is defined via the relation

$$E=E_2^c-\frac{\hbar^2\tilde{q}_2^{\,2}}{2m_2a_2^2} . \tag{29}$$

Perturbation expansion of (27) in the vicinity of the conduction-band edges and comparison with the effective-mass condition (28) yields, naturally, values of β and δ in accordance with (24) and (25). To illustrate the asymptotic agreement, we plot in Fig. 1 the exact and effective-mass quantum-well ground-state energies, both

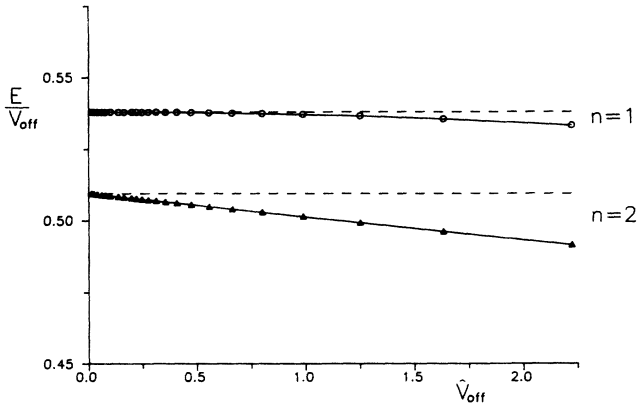

FIG. 1. The quantum-well ground-state energy computed exactly (solid) and approximately (dashed) using effective-mass theory with appropriate boundary conditions for an odd-n ($n=1$) and an even-n ($n=2$) band. Here, $a_2/a_1=1.05$ and $V_{\text{off}}=80\hbar^2/2m_0a_2^2p_1^2$. For $n=1$ we choose $\alpha_1=0.5$, $\alpha_2=1$, and use the boundary conditions (4) with $\beta=-1$ and $\delta=0$. For $n=2$ we similarly use $\alpha_1=2$, $\alpha_2=4$, $\beta=1$, and $\delta=-1$. The effective masses are the same in the two cases so the discrepancies between the effective-mass results are due to different boundary conditions only. The ground-state energies are measured from the band edge of material 2 (barrier). Here, $\hat{V}_{\text{off}}=2m_0a_2^2V_{\text{off}}/\hbar^2$ is a dimensionless offset. Data points corresponding to $p_1=6,7,8,\ldots$ are shown. Asymptotic agreement between effective-mass results and exact results is obtained in the zero-offset limit in both cases.

for an *odd-n* and an *even-n* band, as functions of the offset V_{off}.

C. Local potential

The last example we consider is a local potential $v(x)$ localized at a heterointerface between two materials. Again we model the materials as Kronig-Penney lattices, and we choose the local potential to be a square well, i.e.,

$$v(x)=\begin{cases}-V_0 & \text{for } -s_2a_2\le x\le s_1a_1\\ 0 & \text{otherwise.}\end{cases} \tag{30}$$

Here the width parameters s_1 and s_2 are integers. The condition for bound states is[1]

$$\sum_{i=1}^{2}\tilde{\eta}_i\frac{\sin U_i}{a_iB_i}\tan(s_iU_i+\delta_i)=0\ , \tag{31}$$

where in addition to the definitions (10)–(14) we have defined

$$\tan\delta_i=-\frac{\tilde{\eta}_iB_i\sinh v_i}{\eta_ib_i\sin U_i}\ , \tag{32}$$

$$Q_i=[2m_0a_i^2(E-V_i+V_0)/\hbar^2]^{1/2}\ , \tag{33}$$

$$\cos U_i=|\cos Q_i-\alpha_iQ_i^{-1}\sin Q_i|,\quad 0\le U_i\le\pi/2 \tag{34}$$

$$\tilde{\eta}_i=\mathrm{sgn}(\cos Q_i-\alpha_iQ_i^{-1}\sin Q_i)\ , \tag{35}$$

and

$$B_i=Q_i^{-1}\sin Q_i-\alpha_iQ_i^{-2}+\alpha_iQ_i^{-2}\cos Q_i\ . \tag{36}$$

In analogy with the superlattice case, condition (31) can be simplified when V_0 is small and the energy of the bound state is close to both conduction-band edges in question. To lowest nonvanishing order in U_i we have for B_i

$$B_i=\begin{cases}-2\dfrac{m_i}{m_0}, & n \text{ odd}\\[2ex] \dfrac{m_0}{2\pi^2n^2m_i}U_i^2, & n \text{ even}\end{cases} \tag{37}$$

and (31) and (32) reduce to

$$\sum_{i=1}^{2}\frac{U_i}{a_im_i}\tan(s_iU_i+\delta_i)=0\ , \tag{38}$$

$$\tan\delta_i=-\frac{v_i}{U_i} \tag{39}$$

for *odd n*, and

$$\sum_{i=1}^{2}\frac{a_iU_i}{m_i}\tan(s_iU_i+\kappa_i)=0\ , \tag{40}$$

$$\tan\kappa_i=-\frac{1}{\tan\delta_i}=-\frac{v_i}{U_i} \tag{41}$$

for *even n*.

The condition for bound states from effective-mass theory is

$$\sum_{i=1}^{2}m_i^{\beta}\frac{\tilde{Q}_i}{a_i^{2\delta+1}}\tan(s_i\tilde{Q}_i+\tilde{\delta}_i)=0\ , \tag{42}$$

where the new auxiliary variables $\tilde{Q}_i$ and $\tilde{\delta}_i$ are defined via the relations

$$\tan\tilde{\delta}_i=-\tilde{q}_i/\tilde{Q}_i \tag{43}$$

and

$$\tilde{Q}_i=[2m_ia_i^2(E-E_i^c+V_0)/\hbar^2]^{1/2}\ . \tag{44}$$

By setting $\delta=0$ the condition (42) reduces to the one obtained in Ref. 1.

In Ref. 1, it was demonstrated that the auxiliary variables U_i and v_i are close to $\tilde{Q}_i$ and $\tilde{q}_i$, respectively, when both the band offset and V_0 are small. By inspection of the effective-mass condition (42) and the limiting cases (38) and (40) of the exact condition, one observes that asymptotic equivalence only can be achieved if β and δ are chosen as in the superlattice case, namely

$$\beta=-1 \text{ and } \delta=-\tfrac{1}{2}[1+(-1)^n],\quad n=1,2,3,\ldots. \tag{45}$$

III. HEURISTIC ARGUMENT FOR $\beta=-1$ AND $\delta=-\frac{1}{2}[1+(-1)^n]$

The value of δ just obtained is universal in the sense that δ is the same for different situations as long as the same bands are involved. δ, however, is not generally universal, and this is at first glance worrisome since it is not obvious how to generalize to realistic situations. It would be useful if one could obtain some insight into why δ oscillates between 0 and -1 with increasing band index n. Therefore a heuristic explanation is now offered.

In standard effective-mass theory for, e.g., impurity states in *homogeneous* semiconductors, the leading term in the wave function is in the one-dimensional case,[3]

$$\psi(x)=\phi(x)u_{n0}(x)\ . \tag{46}$$

Here, u_{n0} is the Bloch function at the band edge labeled n. If the probability density $|\phi(x)|^2$ should be a coarse-grained representation of $|\psi(x)|^2$, the periodic modulation u_{n0} in (46) must be normalized according to

$$\frac{1}{a}\int_{-a/2}^{a/2}|u_{n0}(t)|^2\,dt=1\ . \tag{47}$$

For the Kronig-Penney conduction bands involved in the discussion in the previous section, the properly normalized Bloch states at the band edges have the form

$$u_{n0}=\sqrt{2}\sin\left[\frac{n\pi x}{a}\right] \tag{48}$$

when the δ-function wells are located at $0,\pm a,\pm 2a,\ldots$.

In the envelope-function approach[4] for semiconductor heterostructures, solutions of the effective-mass equation are found for each constituent material separately, and the envelope functions are matched at the material boundaries. This approach motivates the following argument.

Consider a heterointerface between two Kronig-Penney materials (1 and 2) with unequal lattice constants

a_1 and a_2 (Fig. 2). Continuity of the true wave function ψ and its derivative ψ' requires, when the form (46) is assumed, that

$$\phi_1 u_{n0,1} = \phi_2 u_{n0,2} \tag{49}$$

and

$$\phi_1' u_{n0,1} + \phi_1 u_{n0,1}' = \phi_2' u_{n0,2} + \phi_2 u_{n0,2}' \tag{50}$$

are fulfilled at the heterointerface. For definiteness we assume for the moment that the conduction-band edges in question are of the same type in both materials, i.e., correspond to the same value of n. For *odd* n the value of u_{n0} at the heterointerface is $\sqrt{2}$ independent of the lattice constant (Fig. 2). Condition (49) thus reduces to

$$\phi_1 = \phi_2 , \tag{51}$$

which corresponds to the parameter values $\alpha=0$, $\beta=-1$, and $\delta=0$ [see (4)]. For *even* n, u_{n0} vanishes at the interfaces, and (49) contains no information about the matching conditions for ϕ. Since the interface value of u_{n0}' is inversely proportional to the lattice constant a, however, condition (50) requires

$$\frac{\phi_1}{a_1} = \frac{\phi_2}{a_2} , \tag{52}$$

which by (4) indicates $\alpha=0$, $\beta=-1$, and $\delta=-1$. The discontinuity of u_{n0}' at the interface when $a_1 \neq a_2$ is seen in Fig. 2.

To illustrate further the use of this simple argument, we also consider the case when the two conduction-band edges in question are of different type. When two different *odd-n* bands are involved (e.g., $n_1=1, n_2=3$), the boundary conditions that give asymptotic agreement are the same as for $n_1=n_2$. With two different *even-n* bands, however, one can show that the boundary conditions

$$\frac{n_1}{a_1}\phi_1 = \frac{n_2}{a_2}\phi_2 \tag{53}$$

and

$$\frac{1}{m_1}\frac{a_1}{n_1}\phi_1' = \frac{1}{m_2}\frac{a_2}{n_2}\phi_2' \tag{54}$$

ensure asymptotic agreement between effective-mass results and exact results in the present test cases. The continuity of $(n/a)\phi$ (53) for even n *also* follows from the heuristic argument above. Since $u_{n0}=0$ and $u_{n0}'=\sqrt{2}(n\pi/a)$ at the interface, $(n/a)\phi$ must be continuous in order for (50) to be fulfilled.

Although these simple arguments predict the correct boundary conditions, a word of caution should be given. If, for instance, relation (50) is taken literally for odd n, the condition $\phi_1'=\phi_2'$ is obtained. This erroneous result reflects that the approximate form of the wave function assumed in (46) has limited validity.

When one of the n's is even and the other odd, no choice of boundary conditions seems to secure asymptotic agreement. This indicates that a simple one-band effective-mass theory is insufficient.

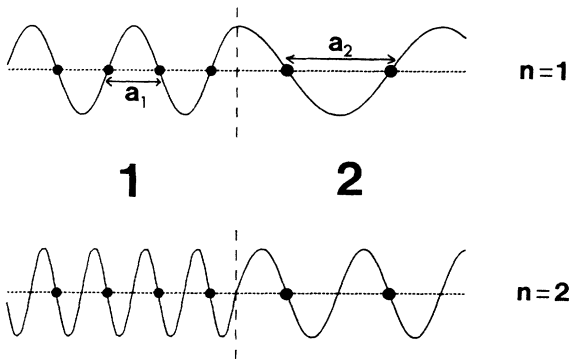

FIG. 2. Matching of Kronig-Penney conduction-band-edge Bloch functions at a heterointerface between material 1 and 2. The interface (dashed) is modeled by joining up two Wigner-Seitz cells corresponding to the two constituent materials. For $n=1$, the two properly normalized Bloch functions match at the interface. For $n=2$, the wave function vanishes and the derivative is discontinuous at the interface. The dots represent δ-function wells.

IV. APPLICATION TO STRAINED HETEROSTRUCTURES

Care must always be taken when applying conclusions reached in one-dimensional models to realistic three-dimensional systems. Nevertheless, such simple models often have provided useful qualitative insights. The present model calculations suggest boundary conditions to use in effective-mass calculations on strained heterostructures.

Let us consider for definiteness a strained quantum well consisting of well material with bulk lattice constant a_W embedded between two thick slabs of barrier material with lattice constant $a_B < a_W$. We focus on well widths less than the so-called critical layer thickness so that a dislocation-free strained layer will be energetically stable.[2] For a sufficiently thin well it is also reasonable to assume that all the strain will be incorporated in the well layer. The well material is forced into the tighter crystal structure of the barrier material in the two in-plane direction, and will relax, i.e., elongate, along the growth direction (Fig. 3). The net strain in the layer plane is given by

$$\epsilon_{\parallel} = \frac{a_B - a_W}{a_W} \tag{55}$$

and similarly in the growth direction

$$\epsilon_{\perp} = \frac{a_W^{\perp} - a_W}{a_W} . \tag{56}$$

Here, $a_W^{\perp}$ denotes the new lattice constant in the growth direction. For tetrahedral semiconductors $\epsilon_{\perp} \simeq -\epsilon_{\parallel}$,[2] and since a_W is set larger than a_B in our example, this indicates $a_W^{\perp} > a_W > a_B$. The difference between the new lat-

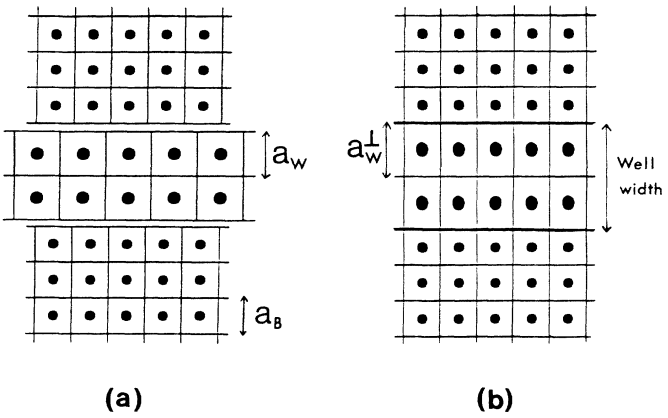

FIG. 3. Schematic illustration of perfect accommodation of strain. The mismatched well material in (a) is squeezed in the in-plane directions and elongated in the growth direction (b).

tice constant in the growth direction ($a_W^\perp$) and the barrier lattice constant (a_B) is therefore approximately twice the difference in pure materials. In effective-mass theory the strained-layer lattice constant to use in the boundary conditions at heterointerfaces is presumably the lattice constant $a_W^\perp$, *not* the lattice constant of the pure material (a_W). This enhances the sensitivity to the choice of boundary conditions.

Which value of δ is appropriate for realistic systems? The Bloch states at conduction-band edges in realistic semiconductor crystals typically have an antibonding nature.[5] The wave function has a node between adjacent atoms and resembles in that respect the $n=2$ case for Kronig-Penney lattices. In Sec. III the value of δ seemed to be governed by the behavior of the band-edge wave function at the heterointerface. This suggests that the *even-n* boundary conditions ($\beta=-1,\delta=-1$) should be used for conduction-band states in strained heterostructures where both conduction-band minima in question are of the same type (e.g., $In_xGa_{1-x}As$-GaAs systems).

A simple one-band effective-mass theory is in general inadequate to describe valence-band states; a multiband description is usually required. However, for important special cases the set of equations simplifies and reduces to simple effective-mass equations for the hole states.[6] Valence-band wave functions at the zone center have a bonding character[5] *without* a node between neighboring atoms and resembles in this respect the $n=1$ case for the Kronig-Penney lattices. This suggests that the *odd-n* boundary conditions, $\beta=-1$ and $\delta=0$, should be used in the effective-mass description of hole states.

Note that the utilization of the boundary conditions prescribed above must be done in addition to including, e.g., strain-induced energy terms from deformation-potential theory in the effective-mass Hamiltonian.[7] Note also that the assumption of abrupt changes in the lattice constant at heterointerfaces is an oversimplification of the situation encountered in many real systems. A more gradual change over a few unit cells can be imagined instead. Since a consecutive series of small changes can be viewed as a gradual change on a coarser scale, an effective-mass treatment involving a nonabrupt position-dependent lattice constant may be applicable to such systems. If so, the present work suggests that the kinetic-energy operator (2), with the choices of δ and β stated above, should be used.

V. SUMMARY

A new effective-mass Hamiltonian for strained heterostructures has been introduced. Through comparisons between results from exact model calculations and effective-mass results, boundary conditions to use at abrupt heterointerfaces have been obtained. A loose qualitative argument, which predicts the right boundary conditions, indicates that the form of the boundary conditions is governed by the behavior of the Bloch wave functions at the band edges in question. Based on qualitative similarities between Kronig-Penney band-edge wave functions and band-edge wave functions in realistic semiconductor crystals, the following boundary conditions for strained heterostructures are proposed:

$$\frac{1}{a}\phi=\text{continuous},\quad \frac{a}{m}\phi'=\text{continuous} \tag{57}$$

for conduction-band states, and

$$\phi=\text{continuous},\quad \frac{1}{m}\phi'=\text{continuous} \tag{58}$$

for valence-band states (*when* a one-band theory is applicable).

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