



# Inclusion of Nonlinear Strain Effects in the Hamiltonian for Nanoscale Semiconductor Structures

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In this paper a general method of treating Hamiltonians of deformed nanoscale semiconductor structures based on a Taylor series expansion<sup>1</sup> is used to derive two second-order approximations with respect to a known deformation, one based on the weak formulation and one based on the strong formulation of the problem. In the case of the strong formulation of the problem appropriate interface boundary conditions are derived. In addition, a second-order approximation with respect to a known strain tensor is derived. As a model example, energies for a one-dimensional Kronig-Penney potential are calculated with an exact, a first-order and a second-order strain Hamiltonian. Also, the more realistic example of a rectangular quantum dot is studied. In this example the strain tensor is found using linear isotropic strain theory and the resulting strain tensor is used to study the influence of including first- and second-order strain contributions in electronic band-structure calculations.

**Keywords:** Strain, Schrödinger Equation, Weak Formulation, Strong Formulation, Taylor Series Expansion.

## 1. THEORY

In order to include the effect of strain in the Hamiltonian for nanoscale semiconductor structures it is necessary to work with the deformation of the system instead of the strain. The relationship between a deformation  $\phi$  and the associated Green-Lagrange-St. Venant strain tensor is given by

$$\epsilon = \frac{1}{2}(\nabla\phi^T\nabla\phi - I) \quad (1)$$

where  $\nabla$  is the gradient on the domain of  $\phi$  and  $I$  is the identity matrix. Here and in the following, coordinates, functions and operators with a superscript  $d$  ( $d$ ) refer to the deformed domain  $\phi(\mathcal{B})$  while coordinates, functions and operators without a superscript refer to the undeformed domain  $\mathcal{B}$  (see Fig. 1).

The strain, and hence the deformation gradient, of a semiconductor heterostructure are usually discontinuous at interfaces. For the strain to be defined away from interfaces the deformation needs to be at least once differentiable away from interfaces. Therefore the following definition of a deformation of a semiconductor heterostructure is necessary.

**Definition 1.** A deformation  $\phi$  is a continuous injective map  $\phi: \mathcal{B} \rightarrow \mathbb{R}^3$  which is once differentiable on  $\mathcal{B} \setminus \Gamma$  with

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both a finite  $C^1$  norm:

$$\|\phi\|_{C^1} = \left\{ \sup_{\mathcal{B} \setminus \Gamma} \left[ \phi_1^2 + \sum_{i=1}^3 \left( \frac{\partial \phi_1}{\partial x_i} \right)^2 + \phi_2^2 + \sum_{i=1}^3 \left( \frac{\partial \phi_2}{\partial x_i} \right)^2 + \phi_3^2 + \sum_{i=1}^3 \left( \frac{\partial \phi_3}{\partial x_i} \right)^2 \right] \right\}^{1/2} \quad (2)$$

and a positive Jacobian determinant, i.e.,  $\inf_{\mathcal{B} \setminus \Gamma} \{\det(\nabla\phi)\} > 0$ , where  $\mathcal{B}$  is an open subset of  $\mathbb{R}^3$ ,  $\Gamma$  is a closed subset of  $\mathcal{B}$  and a union of a finite number of piecewise smooth surfaces (2-dimensional manifolds),  $\phi(\Gamma)$  is closed and the function  $\phi_i$  is the  $i$ 'th component of  $\phi$ , i.e.,  $\phi(x) = (\phi_1(x), \phi_2(x), \phi_3(x))$ . The set  $\mathcal{B}$  is called the reference configuration.

The determination of the deformation for a specific system is outside the scope of this paper. For a discussion of this refer to for example Ref. [2] for the linear isotropic case and to<sup>3,4</sup> for the nonlinear case.

There is freedom of choice with respect to the reference configuration, however, when determining strain in a specific material it is customary to define the strain of the system with respect to an equilibrium configuration (bulk material), i.e., a configuration where the strain energy has a minimum. The materials in a heterostructure are assumed to have been brought into contact by a shrink

Fig. 1.  
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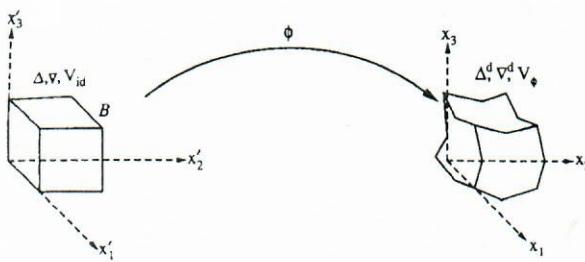


Fig. 1. A sketch of a deformation with related operators and functions used.

fit, i.e., the materials were expanded or shrunk by a homogeneous deformation so that they all had the same lattice lengths when they were brought into contact (see Ref. [2]). This assumption is made to ensure that the atomic bonds between different materials match at interfaces. As a consequence, it makes sense to choose the configuration where all the materials have the same lattice lengths as the reference configuration. Although the choice of reference configuration has no influence on the theory it is important when writing down the Hamiltonian for a specific system as will be seen in Section 2.2.

Assuming that an electron in the system deformed by  $\phi$  is subject to the potential  $V_\phi$ , the Hamiltonian of the deformed system, referred to as the deformed Hamiltonian, is given by:

$$H_\phi = -\frac{\hbar^2}{2m} \Delta^d + V_\phi \quad (3)$$

where  $m$  is the mass of the electron,  $\hbar$  is Planck constant divided by  $2\pi$  and  $\Delta^d$  is the Laplace operator. The potential  $V_\phi$  takes into account the presence of the atoms and the other electrons in the structure. In this paper the spin-orbit contribution is neglected. As a consequence, the potential is just a function  $V_\phi: \phi(\mathcal{B}) \rightarrow \mathbb{R}$ . For a discourse of the inclusion of strain in the Hamiltonian including the spin-orbit contribution consult Ref. [1].

In what follows we assume that the domain of the deformed Hamiltonian is the Sobolev space  $H^2(\phi(\mathcal{B}))$  and that the potential is given such that  $H_\phi \psi \in \mathcal{L}^1(\phi(\mathcal{B}))$  for any  $\psi \in H^2(\phi(\mathcal{B}))$ . The allowed energies  $E$  and associated wave functions  $\psi^d$  are found by solving the eigenvalue equation:

$$H_\phi \psi^d = E \psi^d \quad (4)$$

The deformation is normally reasonably small in the sense that the displacement vector field  $d(x) = \phi(x) - x$  is small. As a consequence, it makes sense to use a Taylor series expansion in order to arrive at an approximate Hamiltonian written in terms of the undeformed system and the deformation. The main advantage of this is that the main part of the approximate Hamiltonian will be more symmetric in the sense that locally the main part will be given by the Hamiltonian of the undeformed bulk material and the rest is a small perturbation that takes into account the deformation of the system. This ensures that

unstrained models such as  $k \cdot p$  theory<sup>5</sup> can be used where the strain is treated as a perturbation. Since the deformation is not once differentiable over the whole domain it is necessary to use the weak formulation of the problem, i.e., the allowed energies and associated wave functions are found by solving:

$$\int_{\phi(\mathcal{B})} (\eta^d)^* (H_\phi - E) \psi^d d^3 x^d = 0 \quad (5)$$

for all  $\eta^d \in C_c^\infty(\phi(\mathcal{B}), \mathbb{C})$  (smooth functions with compact support, see e.g. Ref. [6]). In order to use a Taylor series expansion this problem needs to be written with respect to the undeformed domain  $\mathcal{B}$ . For convenience the following expressions are introduced:

$$\mathbf{K}^d(\phi)(\eta^d, \psi^d) = -\frac{\hbar^2}{2m} \int_{\phi(\mathcal{B})} (\eta^d)^* \Delta^d \psi^d d^3 x^d \quad (6)$$

$$\mathbf{V}^d(\phi)(\eta^d, \psi^d) = \int_{\phi(\mathcal{B})} (\eta^d)^* V_\phi \psi^d d^3 x^d \quad (7)$$

and

$$\begin{aligned} \mathbf{W}_\phi^d(\eta^d, \psi^d; E) &= \mathbf{K}^d(\phi)(\eta^d, \psi^d) + \mathbf{V}^d(\phi)(\eta^d, \psi^d) \\ &\quad - \int_{\phi(\mathcal{B})} (\eta^d)^* E \psi^d d^3 x^d \end{aligned} \quad (8)$$

Equation (5) is then given by:

$$\mathbf{W}_\phi^d(\eta^d, \psi^d; E) = 0 \quad (9)$$

Integrating by parts and using that  $\eta$  has compact support, Eq. (6) becomes

$$\mathbf{K}^d(\phi)(\eta^d, \psi^d) = \frac{\hbar^2}{2m} \int_{\phi(\mathcal{B})} \frac{\partial \eta^{d*}}{\partial x_i} \frac{\partial \psi^d}{\partial x_i} d^3 x^d \quad (10)$$

Restricting the integral to  $\phi(\mathcal{B} \setminus \Gamma)$  for the chain rule to apply (this is possible because  $\phi(\Gamma)$  has measure zero (zero volume)), changing coordinates and using the chain rule it is found that

$$\begin{aligned} \mathbf{K}^d(\phi)(\eta^d, \psi^d) &= \frac{\hbar^2}{2m} \int_{\mathcal{B} \setminus \Gamma} [F^{-1} \circ \phi]_{ji} \frac{\partial(\eta^d \circ \phi)^*}{\partial x_j} \\ &\quad \times [F^{-1} \circ \phi]_{ki} \frac{\partial \psi^d \circ \phi}{\partial x_k} \det F d^3 x \end{aligned} \quad (11)$$

where  $F = \nabla \phi$  is the deformation gradient and Einstein's summation convention is used, i.e., summation over repeated indices, e.g.,  $a_i b_i = \sum_{i=1}^3 a_i b_i$ . Rearranging, Eq. (11) becomes

$$\begin{aligned} \mathbf{K}^d(\phi)(\eta^d, \psi^d) &= \frac{\hbar^2}{2m} \int_{\mathcal{B} \setminus \Gamma} [(F^{-1} \circ \phi)(F^{-1} \circ \phi)^T]_{ij} \\ &\quad \times \frac{\partial(\eta^d \circ \phi)^*}{\partial x_i} \frac{\partial \psi^d \circ \phi}{\partial x_j} \det F d^3 x \end{aligned} \quad (12)$$

Changing coordinates in the expression for the potential (Eq. 7) and the last term of expression (8) it is seen that

written with respect to the domain  $\mathcal{B}$  Eq. (9) becomes

$$\mathbf{W}_\phi(\eta^d \circ \phi, \psi^d \circ \phi; E) = 0 \quad (13)$$

where

$$\begin{aligned} \mathbf{W}_\phi(\eta^d \circ \phi, \psi^d \circ \phi; E) \\ = \mathbf{K}_\phi(\eta^d \circ \phi, \psi^d \circ \phi) + \mathbf{V}_\phi(\eta^d \circ \phi, \psi^d \circ \phi) \\ - \int_{\mathcal{B}} (\eta^d \circ \phi)^* E \psi^d \circ \phi \det F d^3x \end{aligned} \quad (14)$$

$$\begin{aligned} \mathbf{K}_\phi(\eta^d \circ \phi, \psi^d \circ \phi) &= \frac{\hbar^2}{2m} \int_{\mathcal{B} \setminus \Gamma} [(F^{-1} \circ \phi)(F^{-1} \circ \phi)^T]_{ij} \\ &\times \frac{\partial(\eta^d \circ \phi)^*}{\partial x_i} \frac{\partial \psi^d \circ \phi}{\partial x_j} \det F d^3x \end{aligned} \quad (15)$$

and

$$\mathbf{V}_\phi(\eta^d \circ \phi, \psi^d \circ \phi) = \int_{\mathcal{B}} (\eta^d \circ \phi)^* V_\phi \circ \phi \psi^d \circ \phi \det F d^3x \quad (16)$$

On the basis of these definitions, it can be shown that the weak formulation of the problem is equivalent to solving:<sup>1</sup>

$$\mathbf{W}_\phi(\eta, \psi; E) = 0 \quad (17)$$

for all  $\eta \in C_c^\infty(\mathcal{B}, \mathbb{C})$ , where  $\psi \in H^2(\mathcal{B})$ . The Taylor series expansion of  $\mathbf{W}_\phi$  can be found and it is given by

$$\mathbf{W}_\phi \approx \mathbf{W}_{id} + \mathbf{W}^{(1)}(\phi - id) + \mathbf{W}^{(2)}(\phi - id, \phi - id) \quad (18)$$

where

$$\begin{aligned} \mathbf{W}^{(1)}(\phi - id)(\eta, \psi; E) \\ = -\frac{\hbar^2}{2m} \int_{\mathcal{B} \setminus \Gamma} [F + F^T - 2I]_{ij} \frac{\partial \eta^*}{\partial x_i} \frac{\partial \psi}{\partial x_j} \\ - \frac{\partial \eta^*}{\partial x_i} \frac{\partial \psi}{\partial x_i} \text{Tr}(F - I) d^3x + \int_{\mathcal{B}} \eta^* (DV_{id} \cdot (\phi - id) \\ + (V_{id} - E) \text{Tr}(F - I)) \psi d^3x \end{aligned} \quad (19)$$

$$\begin{aligned} \mathbf{W}^{(2)}(\phi - id, \phi - id)(\eta, \psi; E) \\ = \frac{\hbar^2}{2m} \int_{\mathcal{B} \setminus \Gamma} [(F - I)^2 + (F^T - I)^2 + (F - I)(F - I)^T]_{ij} \\ \times \frac{\partial \eta^*}{\partial x_i} \frac{\partial \psi}{\partial x_j} d^3x - \frac{\hbar^2}{2m} \int_{\mathcal{B} \setminus \Gamma} [F + F^T - 2I]_{ij} \text{Tr}(F - I) \\ \times \frac{\partial \eta^*}{\partial x_i} \frac{\partial \psi}{\partial x_j} d^3x + \frac{\hbar^2}{2m} \int_{\mathcal{B} \setminus \Gamma} \frac{\partial \eta^*}{\partial x_i} \frac{\partial \psi}{\partial x_i} \text{Tr}([F - I]_{co}) d^3x \\ + \frac{1}{2} \int_{\mathcal{B}} \eta^* D^2 V_{id} \cdot (\phi - id, \phi - id) \psi d^3x \\ + \int_{\mathcal{B}} \eta^* (DV_{id} \cdot (\phi - id) \text{Tr}(F - I) \\ + (V_{id} - E) \text{Tr}([F - I]_{co})) \psi d^3x \end{aligned} \quad (20)$$

the function  $id$  is the identity function on  $\mathcal{B}$ , i.e.,  $id(x) = x$ , the matrix  $A_{co}$  is the matrix of cofactors of  $A$  and  $DV_{id}$  and  $D^2 V_{id}$  are the first and second Gâteaux derivatives of  $V_{id}$  at  $id$ , respectively. The only assumptions needed in order for the Taylor series expansion to exist are that the potential is Gâteaux differentiable in a convex neighborhood of  $id$  including  $\phi$  and that it is well-behaved. For a detailed derivation of this result refer to Ref. [1], where it is also specified what the term well-behaved entails. Higher-order approximate models can easily be derived by including higher-order terms in the Taylor series expansion. It should be noted that the problem is still a linear eigenvalue problem as the deformation gradient appears in the coefficients of the Hamiltonian only.

The question of whether or not the solutions to the approximate model will be close to the solutions of the exact problem is outside the scope of this paper. However, it is expected, as is usually done in perturbation theories, that approximate solutions will be close to exact solutions. In practice, note that a linear strain term in the Hamiltonian has successfully been used to model the effect of strain for decades (see, e.g., [7]).

### 1.1. Strong Form with Interface Boundary Conditions

In many instances it can be advantageous to have a strong formulation of a problem as this enables one to use other schemes to solve the problem. In order to convert the problem to a strong formulation the assumption that the deformation  $\phi$  is twice differentiable on  $\mathcal{B} \setminus \Gamma$  is needed. Using this assumption and integrating by parts the kinetic term  $\mathbf{K}_\phi$  gives:

$$\begin{aligned} \mathbf{K}_\phi(\eta, \zeta) \\ = -\frac{\hbar^2}{2m} \int_{\mathcal{B} \setminus \Gamma} \eta^* \frac{\partial}{\partial x_i} \left[ \det F [(F^{-1} \circ \phi)(F^{-1} \circ \phi)^T]_{ij} \frac{\partial \zeta}{\partial x_j} \right] d^3x \\ + \frac{\hbar^2}{2m} \int_{\Gamma} n_i \left\{ \left( [(F^{-1} \circ \phi)(F^{-1} \circ \phi)^T]_{ij} \eta^* \frac{\partial \zeta}{\partial x_j} \det F \right)_{m1} \right. \\ \left. - \left( [(F^{-1} \circ \phi)(F^{-1} \circ \phi)^T]_{ij} \eta^* \frac{\partial \zeta}{\partial x_j} \det F \right)_{m2} \right\} dS \end{aligned} \quad (21)$$

where the subscripts  $m1$  and  $m2$  symbolize that the expression in brackets is found as the limit taken from the region that the normal vector points out of and into, respectively,  $\vec{n} = (n_1, n_2, n_3)$  is a unit normal vector field on the interface  $\Gamma$  and  $\int_{\Gamma} f dS$  is the surface integral over  $\Gamma$ . To get this result it has also been used that

$$\frac{\partial}{\partial x_i} (F_{ik}^{-1} \det F) = \frac{\partial}{\partial x_i} ([F_{co}]_{ki}) = 0 \quad (22)$$

for  $k = 1, 2, 3$ . From this it can be seen that the weak formulation is equivalent to solving

$$\hat{H}_\phi \psi = E \psi \quad (23)$$

on  $\mathcal{B} \setminus \Gamma$ , where

$$\begin{aligned}\widehat{H}_\phi = & -\frac{\hbar^2}{2m \det F} \frac{\partial}{\partial x_i} \left[ \det F [F^{-1} \circ \phi](F^{-1} \circ \phi)^T]_{ij} \frac{\partial}{\partial x_j} \right] \\ & + V_\phi \circ \phi\end{aligned}\quad (24)$$

subject to the interface boundary conditions

$$\begin{aligned}n_i \left( [F^{-1} \circ \phi](F^{-1} \circ \phi)^T]_{ij} \frac{\partial \psi}{\partial x_j} \det F \right)_{m1} \\ = n_i \left( [F^{-1} \circ \phi](F^{-1} \circ \phi)^T]_{ij} \frac{\partial \psi}{\partial x_j} \det F \right)_{m2}\end{aligned}\quad (25)$$

The second-order Taylor series expansion of  $\widehat{H}_\phi$  is given by

$$\widehat{H}_\phi \approx \widehat{H}_{id} + D^{(1)} \cdot (\phi - id) + D^{(2)} \cdot (\phi - id, \phi - id) \quad (26)$$

where

$$\widehat{H}_{id} = -\frac{\hbar^2}{2m} \Delta + V_{id} \quad (27)$$

$$\begin{aligned}D^{(1)} \cdot (\phi - id) = & \frac{\hbar^2}{2m} \left\{ [F + F^T - 2I]_{jk} \frac{\partial}{\partial x_j} \frac{\partial}{\partial x_k} \right. \\ & + \sum_{i=1}^3 \sum_{k=1}^3 \frac{\partial}{\partial x_i} ([F - I]_{ki}) \frac{\partial}{\partial x_k} \Big\} \\ & + DV_{id} \cdot (\phi - id)\end{aligned}\quad (28)$$

$$\begin{aligned}D^{(2)} \cdot (\phi - id, \phi - id) = & -\frac{\hbar^2}{2m} \left\{ [(F - I)(F - I)^T]_{jk} \frac{\partial}{\partial x_j} \frac{\partial}{\partial x_k} \right. \\ & + [(F - I)]_{ji} \frac{\partial}{\partial x_j} ([F - I]_{ki}) \frac{\partial}{\partial x_k} \\ & + [(F - I)^2 + (F^T - I)^2]_{jk} \frac{\partial}{\partial x_j} \frac{\partial}{\partial x_k} \\ & + \frac{\partial}{\partial x_i} [(F - I)^2]_{ki} \frac{\partial}{\partial x_k} \Big\} \\ & + \frac{1}{2} D^2 V_{id} \cdot ((\phi - id), (\phi - id))\end{aligned}\quad (29)$$

Refer to Ref. [1] for a detailed derivation of this result. The second-order Taylor series expansion of the interface boundary conditions takes the form:

$$[R\psi]_{m1} = [R\psi]_{m2} \quad (30)$$

where

$$\begin{aligned}R = & n_i \left\{ \frac{\partial}{\partial x_i} - [F + F^T - 2I]_{ij} \frac{\partial}{\partial x_j} + \text{Tr}(F - I) \frac{\partial}{\partial x_i} \right. \\ & + [(F - I)^2 + (F^T - I)^2 + (F - I)(F^T - I)]_{ij} \frac{\partial}{\partial x_j} \\ & + \text{Tr}(F - I)[F + F^T - 2I]_{ij} \frac{\partial}{\partial x_j} + \text{Tr}([F - I]_{co}) \frac{\partial}{\partial x_i} \Big\}\end{aligned}\quad (31)$$

## 1.2. Deformed Hamiltonian in Terms of Strain

In many cases the strain tensor is known but the deformation gradient is not. For instance, this is the case when the strain is found using the linear isotropic continuum mechanical model, see, e.g., Stier et al.<sup>8</sup> and references therein. Under those circumstances it is advantageous to have a model depending directly on the strain tensor instead of the deformation gradient. This is possible in the case considered in this paper. However, it is not always possible, e.g., if the spin-orbit correction is included it is no longer possible to write out the problem in terms of the nonlinear strain tensor. In the following it is shown how to derive approximations directly with respect to the strain tensor for the case considered in this paper.

From the definition of the strain, Eq. (1), it can be found that

$$F^{-1}[F^{-1}]^T = (2\epsilon + I)^{-1} \quad (32)$$

and

$$\det F = \sqrt{\det(2\epsilon + I)} \quad (33)$$

It is now seen that the kinetic and potential parts are given by

$$\begin{aligned}\widehat{\mathbf{K}}_\epsilon(\eta, \zeta) & \equiv \mathbf{K}_\phi(\eta, \zeta) \\ & = \frac{\hbar^2}{2m} \int_{\mathcal{B} \setminus \Gamma} [(2\epsilon + I)^{-1}]_{ij} \frac{\partial \eta^*}{\partial x_i} \frac{\partial \zeta}{\partial x_j} \sqrt{\det(2\epsilon + I)} d^3 x\end{aligned}\quad (34)$$

and

$$\widehat{\mathbf{V}}_\epsilon(\eta, \zeta) \equiv \mathbf{V}_\phi(\eta, \zeta) = \int_{\mathcal{B}} \eta^* V_\phi \zeta \sqrt{\det(2\epsilon + I)} d^3 x \quad (35)$$

In Eq. (35) it is assumed that the potential on the deformed domain ( $V_\phi$ ) can be written directly with respect to the strain and  $V_\epsilon \equiv V_\phi$ . If a second-order Taylor series expansion of the weak functional:

$$\begin{aligned}\widehat{\mathbf{W}}_\epsilon(\eta, \psi; E) & \equiv \mathbf{W}_\phi(\eta, \psi; E) = \widehat{\mathbf{K}}_\epsilon(\eta, \zeta) + \widehat{\mathbf{V}}_\epsilon(\eta, \zeta) \\ & - \int_{\mathcal{B}} \eta^* E \psi \sqrt{\det(2\epsilon + I)} d^3 x\end{aligned}\quad (36)$$

is made with respect to  $\epsilon$  around the zero tensor (no strain) it is found that

$$\widehat{\mathbf{W}}_\epsilon \approx \widehat{\mathbf{W}}_0 + \widehat{\mathbf{W}}^{(1)}(\epsilon) + \widehat{\mathbf{W}}^{(2)}(\epsilon, \epsilon) \quad (37)$$

where

$$\widehat{\mathbf{W}}_0(\eta, \psi; E) = \frac{\hbar^2}{2m} \int_{\mathcal{B} \setminus \Gamma} \frac{\partial \eta^*}{\partial x_i} \frac{\partial \psi}{\partial x_i} d^3 x + \int_{\mathcal{B}} \eta^* (V_0 - E) \psi d^3 x \quad (38)$$

$$\begin{aligned}\widehat{\mathbf{W}}^{(1)}(\epsilon)(\eta, \psi; E) \\ = -\frac{\hbar^2}{2m} \int_{\mathcal{B} \setminus \Gamma} 2\epsilon_{ij} \frac{\partial \eta^*}{\partial x_i} \frac{\partial \psi}{\partial x_j} - \frac{\partial \eta^*}{\partial x_i} \frac{\partial \psi}{\partial x_i} \text{Tr}(\epsilon) d^3 x \\ + \int_{\mathcal{B}} \eta^* (DV_0 \cdot (\epsilon) + (V_0 - E) \text{Tr}(\epsilon)) \psi d^3 x\end{aligned}\quad (39)$$

and

$$\begin{aligned} \widehat{\mathbf{W}}^{(2)}(\epsilon, \epsilon)(\eta, \psi; E) &= \frac{\hbar^2}{2m} \int_{\mathcal{B} \setminus \Gamma} [4\epsilon^2 - 2\epsilon \text{Tr}(\epsilon)]_{ij} \frac{\partial \eta^*}{\partial x_i} \frac{\partial \psi}{\partial x_j} + \frac{\partial \eta^*}{\partial x_i} \frac{\partial \psi}{\partial x_i} (2\text{Tr}(\epsilon_{co}) \\ &\quad - \frac{1}{2} [\text{Tr}(\epsilon)]^2) d^3x + \frac{1}{2} \int_{\mathcal{B}} \eta^* (D^2 V_0 \cdot (\epsilon, \epsilon) \psi \\ &\quad + 2DV_0 \cdot (\epsilon) \text{Tr}(\epsilon) + (V_0 - E)(4\text{Tr}(\epsilon_{co}) \\ &\quad - [\text{Tr}(\epsilon)]^2)) \psi d^3x \end{aligned} \quad (40)$$

### 1.2.1. One Band Model

As a special case the one band model for the conduction band electrons is investigated. For zinc-blende materials the deformed Hamiltonian of a conduction-band electron is given by

$$H_\epsilon = -\nabla^d \frac{\hbar^2}{2m_c} \nabla^d + V_\epsilon^{kp} \circ \phi^{-1} \quad (41)$$

where  $m_c$  is the effective mass,  $V_\epsilon^{kp}: \mathcal{B} \rightarrow \mathbb{R}$  is the function:  $V_\epsilon^{kp}(x) = V_\epsilon^{kp,i}(x)$  for  $x$  in material  $i$

$$\begin{aligned} V_\epsilon^{kp,i}(x) &\approx \frac{\hbar^2}{2m} (2\epsilon(x) + I)^{-1} \int_{\phi_0^{(i)}(\Omega_c^{(i)})} \frac{\partial U_S^{(i)*}}{\partial x_i}(x_0) \\ &\quad \times \frac{\partial U_S^{(i)}}{\partial x_j}(x_0) d^3x_0 + \int_{\phi_0^{(i)}(\Omega_c^{(i)})} U_S^{(i)}(x_0)^* V_\epsilon^{(i)} \\ &\quad \times (\phi(x_0)) U_S^{(i)}(x_0) d^3x_0 \end{aligned} \quad (42)$$

$\Omega_c^{(i)}$  is a primitive lattice cell,  $V_\epsilon^{(i)}$  is the deformed crystal potential of material  $i$ , the function  $U_S^{(i)}$  is the conduction band zone-center solution for the homogeneously deformed bulk material and  $\phi_0^{(i)}$  is the homogeneous transformation that ensures that material  $i$  has the same lattice constant as all the other materials in the reference configuration (remembering that some of the materials are homogeneously deformed in the reference configuration, see Fig. 2). The derivation of this result is outside the scope of this paper and will appear in a forthcoming paper. It is assumed for simplicity that the effective mass is independent of the strain although taking into account a strain-dependent effective mass is possible (and natural) in the general case. In the following tilded ( $\tilde{\cdot}$ ) coordinates, functions and operators refer to the bulk material

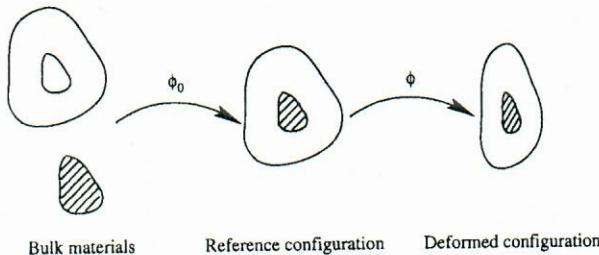


Fig. 2. A sketch of the different configurations.

configuration (see Fig. 2). The homogeneous transformation  $\phi_0^{(i)}$  is given by

$$\phi_0^{(i)}(\tilde{x}) = b^{(i)} \tilde{x} \quad (43)$$

for  $\tilde{x}$  in material  $i$ , where

$$b^{(i)} = \frac{a^{\text{ref}}}{a^{(i)}} \quad (44)$$

the constant  $a^{(i)}$  is the lattice constant of material  $i$  and  $a^{\text{ref}}$  is the lattice constant of the reference configuration. To relate Eq. (42) to bulk material parameters it is assumed that  $V_\epsilon^{(i)} \circ \phi = V_0^{(i)}$  and  $V_0^{(i)} \circ \phi_0^{(i)} = V^{\text{bulk}, i}$ , where  $V^{\text{bulk}, i}$  is the crystal potential of the bulk materials. In this case it is evident that the conduction band zone center solution for the homogeneously deformed bulk material is given by

$$U_S^{(i)}(x_0) = \frac{U_S^{\text{bulk}, i}(\frac{x_0}{b^{(i)}})}{\sqrt{\det(\tilde{\nabla}\phi_0)}} \quad (45)$$

where  $U_S^{\text{bulk}, i}$  is the zone center solution for the undeformed bulk material. The determinant in the denominator is needed in order for the zone center solution to be normalized. Using Eq. (45), it can be shown that

$$\begin{aligned} V_\epsilon^{(i)}(x) &\approx -\frac{a_c^{(i)}}{2[b^{(i)}]^2} \text{Tr}((2\epsilon(x) + I)^{-1}) \\ &\quad + \int_{\Omega_c^{(i)}} U^{\text{bulk}, i}(\tilde{x})^* V^{\text{bulk}, i}(\tilde{x}) U_S^{\text{bulk}, i}(\tilde{x}) d^3\tilde{x} \end{aligned} \quad (46)$$

where

$$a_c^{(i)} = -\frac{2}{m} \sum_{\nu \in \Gamma_{15}} p_{S\nu}^{(i)} p_{\nu S}^{(i)} \quad (47)$$

the sum runs over all  $\Gamma_{15}$  zone-center states (for zinc-blende) and

$$p_{S\nu}^{(i)} = -i\hbar \int_{\Omega_c^{(i)}} [U_S^{\text{bulk}, i}]^* \frac{\partial}{\partial \tilde{x}_1} U_{\nu}^{\text{bulk}, i} d^3\tilde{x} \quad (48)$$

The second-order Taylor series expansion of the weak formulation now takes the form given in Eq. (37) with the electron mass  $m$  replaced with the effective mass  $m_c$ ,

$$DV_0 \cdot (\epsilon) = \frac{a_c^{(i)}}{[b^{(i)}]^2} \text{Tr}(\epsilon) \quad (49)$$

and

$$D^2 V_0 \cdot (\epsilon, \epsilon) = -\frac{2a_c^{(i)}}{[b^{(i)}]^2} \text{Tr}(\epsilon^2) \quad (50)$$

where  $a_c$  is a step function with value  $a_c^{(i)}$  in material  $i$ . The constants  $a_c^{(i)}$  are called deformation potentials and can be found in literature, e.g., Ref. [9]. There is still one material parameter that has to be related to bulk parameters available in literature:

$$\widetilde{V}^{(i)} = \int_{\Omega_c} [U_S^{\text{bulk}, i}]^* V_0^{\text{bulk}, i} U_S^{\text{bulk}, i} d^3\tilde{x} \quad (51)$$

from Eq. (46). This parameter can be related to the bulk conduction band edge energy of material  $i$ , denoted  $E_c^{(i)}$ .

This energy is given by

$$\begin{aligned} E_c^{(i)} &= \int_{\Omega_c} \frac{\hbar^2}{2m} \frac{\partial U_S^{(i)*}}{\partial \tilde{x}_i} \frac{\partial U_S^{(i)}}{\partial \tilde{x}_i} + [U_S^{(i)*}]^* V_0^{\text{bulk}, i} U_S^{(i)} d^3 \tilde{x} \\ &= -\frac{3a_c^{(i)}}{2} + \tilde{V}^{(i)} \end{aligned} \quad (52)$$

so that

$$\tilde{V}^{(i)} = E_c^{(i)} + \frac{3a_c^{(i)}}{2} \quad (53)$$

## 2. EXAMPLES

### 2.1. Strained Kronig-Penney Potential

As an example of the applicability of the second-order strain Hamiltonian, Eq. (26), results for a one-dimensional strained Kronig-Penney potential are presented here. The unstrained Kronig-Penney potential is given by

$$V_{\text{id}}(x) = \frac{3\pi\hbar^2}{2ma} \sum_{n=-N}^N \delta(x - na) \quad (54)$$

for  $x \in [-Na, Na] = \mathcal{B}$ , where  $N \in \mathbb{N}$ ,  $a \in ]0, \infty[$  is the lattice constant and  $\delta$  is the Dirac-delta function. In addition to this, periodic boundary conditions are imposed. Figure 3 shows the first three energy bands obtained.

Assuming that  $N/10 \in \mathbb{N}$ , the Kronig-Penney potential of a strained domain can be found by deforming the position of the Dirac-delta functions by

$$\phi(x) = x + \mathcal{E}a \sin\left(\frac{2\pi}{10a}x\right) \quad (55)$$

where  $\mathcal{E} \in ]0, 1[$  is the magnitude of the deformation. The strain Hamiltonian is then given by

$$H_\phi = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{3\pi\hbar^2}{2ma} \sum_{n=-N}^N \delta(x - \phi(na)) \quad (56)$$

This Hamiltonian does not satisfy that  $H_\phi \psi \in \mathcal{L}^1(\phi(\mathcal{B}))$ , however, this requirement is not needed when working in

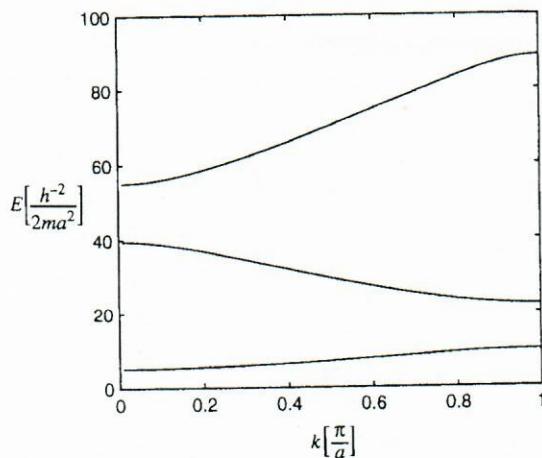


Fig. 3. Energy bands for the undeformed Kronig-Penney potential.

the strong formulation. Also, the weak formulation could easily be extended to handle this kind of potential.

Firstly, using the Bloch theorem the eigenfunctions can be written as  $\psi^d(x^d) = e^{ikx^d} u_k(x^d)$ , where  $k = \frac{\pi m}{Na}$  for  $m \in \mathbb{Z}$  and  $u_k(x^d)$  is periodic with period  $10a$ . Inserting this in the eigenvalue equation  $H_\phi \psi^d = E \psi^d$  produces an equation for  $u_k(x^d)$  with  $k$  as a parameter. This equation can be solved by finding the solutions on the intervals between the delta functions and then imposing the right interface boundary conditions at the positions of the delta functions. This produces a homogeneous matrix system and in order for a non-trivial solution to exist the coefficient matrix of this system of equations must have a determinant equal to zero. The solutions to this nonlinear equation with respect to the eigenvalues give the possible energy levels for a given  $k$ .

The second-order strain Hamiltonian is found by using the deformation to transform the strain Hamiltonian into an operator with functions defined on  $\mathcal{B}$  as domain and then making the Taylor expansion. For the potential in Eq. (56) it is found that

$$\begin{aligned} V_\phi \circ \phi(x) &= \frac{3\pi\hbar^2}{2ma} \sum_{n=-N}^N \delta(\phi(x) - \phi(na)) \\ &= \frac{3\pi\hbar^2}{2ma} \sum_{n=-N}^N \frac{\delta(x - na)}{F(na)} \end{aligned} \quad (57)$$

where  $F(x_0) = \frac{\partial \phi}{\partial x}|_{x_0} = 1 + \frac{2\pi\mathcal{E}}{10a} \cos(\frac{2\pi}{10a}x_0)$ . The second-order strain Hamiltonian in the strong formulation is then given by

$$\begin{aligned} \tilde{H}_\phi &\approx \frac{\hbar^2}{2m} (-1 + 2(F-1) - 3(F-1)^2) \frac{\partial^2}{\partial x^2} \\ &+ \frac{\hbar^2}{2m} \left( \frac{\partial(F-1)}{\partial x} - (F-1) \frac{\partial(F-1)}{\partial x} - \frac{\partial(F-1)^2}{\partial x} \right) \frac{\partial}{\partial x} \\ &+ \frac{3\pi\hbar^2}{2ma} \sum_{n=-N}^N (\delta(x - na)(1 - (F-1) + (F-1)^2)) \end{aligned} \quad (58)$$

Note that the deformation is smooth so no interface boundary conditions have to be imposed as a consequence of the deformation.

The solutions to the eigenvalue equation for this Hamiltonian have been found using the finite element method. In Figure 4, results are shown for the unstrained, strained exact, strained first-order and strained second-order Taylor expansions for  $\mathcal{E} = 0.2$ . Here it is seen that there is almost no difference between the second-order and the exact energy bands, whereas there are clear differences between the first-order and the exact energy bands. To make this comparison more precise calculations have been made for different  $\mathcal{E}$  values at the zone center. In Figure 5, the difference between the energy of the first state calculated with the exact Hamiltonian and the first- and second-order approximations is shown as a function of  $\epsilon$  and the maximum Green-Lagrange-St. Venant strain. The errors of the

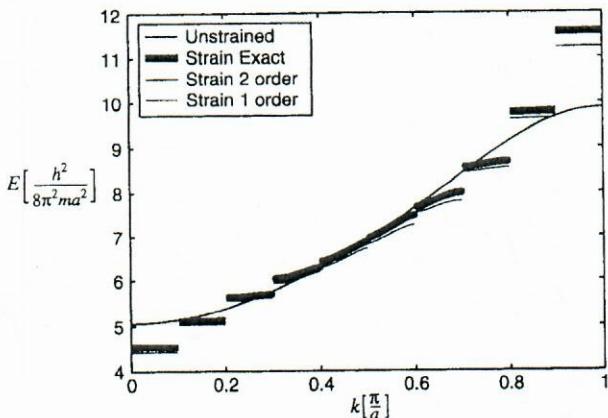


Fig. 4. Energy bands for the potential of the strained Kronig-Penney model for  $\epsilon = 0.2$ .

first- and second-order Hamiltonians are given by

$$\text{Error}^x = \left| \frac{E_1^{\text{Exact}} - E_1^x}{E_1^{\text{Exact}}} \right| \quad (59)$$

where  $x = 1\text{st}, 2\text{nd}$  and  $E_1^{\text{Exact}}$ ,  $E_1^{\text{1st}}$  and  $E_1^{\text{2nd}}$  are the energy of the first state calculated with the exact, first-order and second-order Hamiltonians, respectively.

The Green-Lagrange-St. Venant strain is given by

$$\begin{aligned} \epsilon(x_0) &= \frac{1}{2}(F(x_0)^T F(x_0) - I) \\ &= \frac{2\pi\epsilon}{10} \cos\left(\frac{2\pi}{10a}x_0\right) \left(1 + \frac{\pi\epsilon}{10} \cos\left(\frac{2\pi}{10a}x_0\right)\right) \end{aligned} \quad (60)$$

i.e., the maximum strain is given by  $\frac{2\pi\epsilon}{10}(1 + \frac{\pi\epsilon}{10})$ .

From Figure 5, it can be seen that both the first- and second-order approximations are quite accurate up to a max strain of 7% as the error is less than 1%. It is of

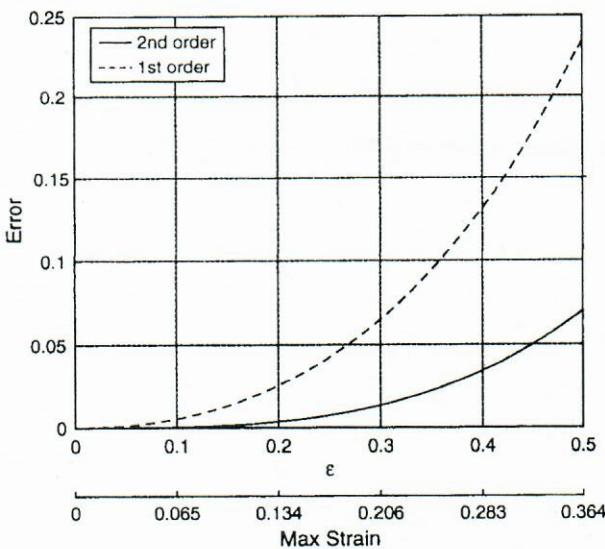


Fig. 5. Error of the first- and second-order strain Hamiltonian at the zone center.

particular interest to note that the second-order approximation has an error of less than 1% for situations with a max strain of up to 18%. This clearly demonstrates that the range of applicability for the second-order approximation is substantially larger than it is for the first-order approximation.

## 2.2. Quantum Dot

In the case of a more realistic structure it is first necessary to find the strain in the system resulting from the lattice mismatch. Assuming that the strain can be described by a linear isotropic model, it can be shown that the stress of one material (the inner material) surrounded by another material (the outer material) is given by:<sup>2,10</sup>

$$\begin{aligned} \sigma_{ij}(\tilde{x}) &= \int_{\partial\Omega_2} \vec{A}_{ij}(\tilde{x} - \tilde{x}_0) d\vec{S}_0 \\ &\quad + \delta_{ij}\delta \frac{3}{((1+\nu^{\text{out}})/E^{\text{out}}) + 2((1-2\nu^{\text{in}})/E^{\text{in}})} \\ &\quad \times \int_{\Omega_2} \delta(\tilde{x} - \tilde{x}_0) d^3\tilde{x}_0 \end{aligned} \quad (61)$$

where  $\delta_{ij}$  is 1 for  $i = j$  and otherwise zero,

$$\vec{A}_{ii}(\tilde{x}_1, \tilde{x}_2, \tilde{x}_3) = \Lambda \frac{\tilde{x}_i}{r^3} \hat{x}_i \quad (62)$$

$$\vec{A}_{12}(\tilde{x}_1, \tilde{x}_2, \tilde{x}_3) = -\Lambda \frac{\tilde{x}_2}{r^3} \hat{x}_1 \quad (63)$$

$$\vec{A}_{13}(\tilde{x}_1, \tilde{x}_2, \tilde{x}_3) = -\Lambda \frac{\tilde{x}_3}{r^3} \hat{x}_1 \quad (64)$$

$$\vec{A}_{23}(\tilde{x}_1, \tilde{x}_2, \tilde{x}_3) = -\Lambda \frac{\tilde{x}_3}{r^3} \hat{x}_2 \quad (65)$$

$$\Lambda = \delta \frac{3}{4\pi} \frac{1}{(1+\nu^{\text{out}})/E^{\text{out}} + 2(1-2\nu^{\text{in}})/E^{\text{in}}} \quad (66)$$

$$\delta = \frac{a^{\text{out}}}{a^{\text{in}}} - 1 \quad (67)$$

$\Omega_2$  is the domain of the inner material,  $r = \sqrt{\tilde{x}_1^2 + \tilde{x}_2^2 + \tilde{x}_3^2}$  and  $\hat{x}_i$  is the unit vector in the direction of the  $\tilde{x}_i$  coordinate axis. The strain is then given by

$$\epsilon_{ij} = \frac{1}{E} \left[ (1+\nu) \sigma_{ij} - \nu \delta_{ij} \sum_n \sigma_{nn} \right] \quad (68)$$

where  $E = E^{\text{in}}$ ,  $\nu = \nu^{\text{in}}$  in the inner material and  $E = E^{\text{out}}$ ,  $\nu = \nu^{\text{out}}$  in the outer material. Here,  $E$  and  $\nu$  denote the bulk modulus and the Poisson ratio, respectively.

The strain found with this method is actually the strain in the system with respect to the undeformed bulk materials, i.e., the bulk material system in Figure 2. However, this is not the strain appearing in the one band model from section 1.2.1. The strain in section 1.2.1 is found with respect to the reference configuration where some of the materials have been homogeneously deformed so that all materials have the same lattice constant. To relate the strain tensors with respect to the two different

configurations observe that

$$\tilde{\epsilon} = \frac{1}{2}(\tilde{\nabla}\tilde{\phi} + [\tilde{\nabla}\tilde{\phi}]^T - 2I) \quad (69)$$

remembering that the linear strain theory is used, where

$$\tilde{\phi} = \phi \circ \phi_0 \quad (70)$$

so that

$$\tilde{\nabla}\tilde{\phi} = b^{(i)}\nabla\phi \quad (71)$$

in material  $i$ . As a consequence it is seen that

$$\tilde{\epsilon}_{ij} = b^{(i)}\epsilon_{ij} + \delta_{ij}(b^{(i)} - 1) \quad (72)$$

in material  $i$ , where  $\epsilon$  is the strain tensor used in section 1.2.1, i.e., with respect to the reference configuration in Figure 2.

As an application of the strain theory the example of a rectangular inclusion of length  $2a$ , width  $2b$  and height  $2c$  is studied, see Figure 6. This structure has been studied by Downes et al.<sup>10</sup> too. By choosing appropriate parameterizations of the surfaces it can be shown that

$$\begin{aligned} \sigma_{ii} &= I_{ii}^{i,+} + I_{ii}^{i,-} + 4\pi\Lambda \int_{\Omega_2} \delta(\tilde{x} - \tilde{x}_0) d^3\tilde{x} \\ \sigma_{12} &= I_{12}^{1,+} + I_{12}^{1,-} \\ \sigma_{13} &= I_{13}^{1,+} + I_{13}^{1,-} \\ \sigma_{23} &= I_{23}^{2,+} + I_{23}^{2,-} \end{aligned} \quad (73)$$

where

$$\begin{aligned} I_{11}^{1,\pm} &= \pm\Lambda(h_1(\mp a, -b, -c) + h_1(\mp a, b, c) \\ &\quad - h_1(\mp a, b, -c) - h_1(\mp a, -b, c)) \\ I_{22}^{2,\pm} &= \pm\Lambda(h_2(-a, \mp b, -c) + h_2(a, \mp b, c) \\ &\quad - h_2(a, \mp b, -c) - h_2(-a, \mp b, c)) \\ I_{33}^{3,\pm} &= \pm\Lambda(h_3(-a, -b, \mp c) + h_3(a, b, \mp c) \\ &\quad - h_3(a, -b, \mp c) - h_3(-a, b, \mp c)) \\ I_{12}^{1,\pm} &= \pm\Lambda(g_{12}(\mp a, -b, -c) + g_{12}(\mp a, b, c) \\ &\quad - g_{12}(\mp a, b, -c) - g_{12}(\mp a, -b, c)) \\ I_{13}^{1,\pm} &= \pm\Lambda(g_{13}(\mp a, -b, -c) + g_{13}(\mp a, b, c) \\ &\quad - g_{13}(\mp a, b, -c) - g_{13}(\mp a, -b, c)) \end{aligned} \quad (74)$$

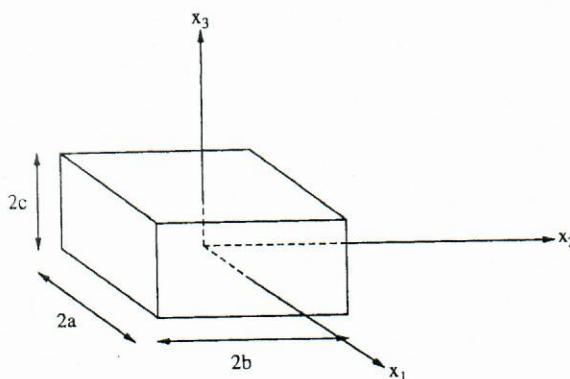


Fig. 6. A rectangular inclusion.

$$\begin{aligned} I_{23}^{2,\pm} &= \pm\Lambda(g_{23}(-a, \mp b, -c) + g_{23}(a, \mp b, c) \\ &\quad - g_{23}(a, \mp b, -c) - g_{23}(-a, \mp b, c)) \end{aligned}$$

and

$$\begin{aligned} h_1(a, b, c) &= \arctan\left(\frac{(\tilde{x}_2 + b)(\tilde{x}_3 + c)}{(\tilde{x}_1 + a)\sqrt{(\tilde{x}_1 + a)^2 + (\tilde{x}_2 + b)^2 + (\tilde{x}_3 + c)^2}}\right) \\ h_2(a, b, c) &= \arctan\left(\frac{(\tilde{x}_1 + a)(\tilde{x}_3 + c)}{(\tilde{x}_2 + b)\sqrt{(\tilde{x}_1 + a)^2 + (\tilde{x}_2 + b)^2 + (\tilde{x}_3 + c)^2}}\right) \\ h_3(a, b, c) &= \arctan\left(\frac{(\tilde{x}_1 + a)(\tilde{x}_2 + b)}{(\tilde{x}_3 + c)\sqrt{(\tilde{x}_1 + a)^2 + (\tilde{x}_2 + b)^2 + (\tilde{x}_3 + c)^2}}\right) \\ g_{12}(a, b, c) &= \ln((\tilde{x}_3 + c) + \sqrt{(\tilde{x}_1 + a)^2 + (\tilde{x}_2 + b)^2 + (\tilde{x}_3 + c)^2}) \\ g_{13}(a, b, c) &= \ln((\tilde{x}_2 + b) + \sqrt{(\tilde{x}_1 + a)^2 + (\tilde{x}_2 + b)^2 + (\tilde{x}_3 + c)^2}) \\ g_{23}(a, b, c) &= \ln((\tilde{x}_1 + a) + \sqrt{(\tilde{x}_1 + a)^2 + (\tilde{x}_2 + b)^2 + (\tilde{x}_3 + c)^2}) \end{aligned} \quad (75)$$

More specifically, the example of a rectangular inclusion of InAs in GaAs is studied. The lattice length of GaAs (InAs) is 5.6533 Å (6.0584 Å) so the relative lattice mismatch is

$$\delta = \frac{a^{\text{out}}}{a^{\text{in}}} - 1 = -0.06687 \quad (76)$$

The Young modulus and Poisson ratio are related to the elastic moduli  $c_{ij}$  according to

$$E = \frac{(c_{11} - c_{12})(c_{11} + 2c_{12})}{c_{11} + c_{12}} \quad (77)$$

and

$$\nu = \frac{c_{12}}{c_{11} + c_{12}} \quad (78)$$

where it is assumed that  $c_{11} - c_{12} = 2c_{44}$  (the isotropic approximation). The elastic moduli  $c_{ij}$  for the two materials are given in Table I together with the Young modulus and Poisson ratio.

In Figure 7, the strain profile relative to the bulk materials ( $\tilde{\epsilon}$ ) is shown along the  $\tilde{x}_3$  axis ( $\tilde{x}_1 = \tilde{x}_2 = 0$ ) for a box with  $a = b = 40$  and  $c = 80$ . Here it is seen that the individual strain components have the largest (and smallest) value around interfaces and that they decay away from interfaces. This is expected as the structure is strained exactly because the two materials are in contact at interfaces. Moreover, it is seen that the outer material is compressed

Table I. Elastic moduli, Young's modulus and Poisson ratio for InAs and GaAs. The elastic moduli are taken from Vurgaftman et al.<sup>9</sup>

	$c_{11}$ [GPa]	$c_{12}$ [GPa]	$c_{44}$ [GPa]	$E$ [GPa]	$\nu$
GaAs	1221	566	600	862.46	0.31673
InAs	832.9	452.6	395.9	514.20	0.35208

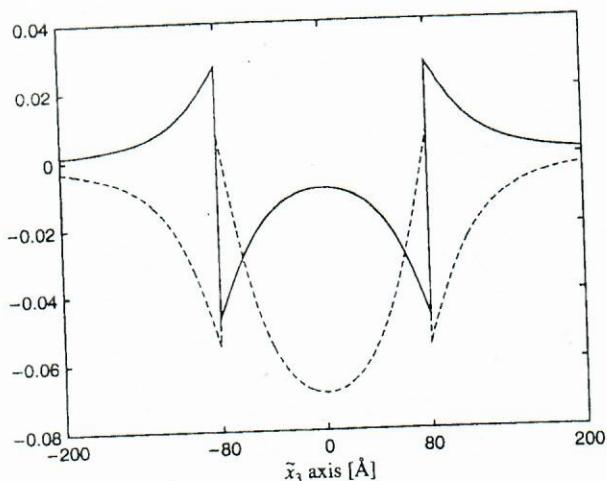


Fig. 7. Strain components with respect to bulk materials for a rectangular inclusion in the  $\tilde{x}_3$ -direction with  $\tilde{x}_1 = 0$  and  $\tilde{x}_2 = 0$  for a structure where  $a = b = 40$  and  $c = 80$ . The solid line is  $\epsilon_{11} = \epsilon_{22}$  and the dashed line is  $\epsilon_{33}$ .

in the  $\tilde{x}_3$  direction, stretched in the  $\tilde{x}_1$  and  $\tilde{x}_2$  direction close to the interface and unstrained sufficiently far away from interfaces. This behaviour is easily understood by imagining that the inner material is trying to expand to its original size (the equilibrium configuration of the bulk material). This will compress the outer material in the  $\tilde{x}_3$  direction and as the interface in the  $\tilde{x}_1$  and  $\tilde{x}_2$  directions is trying to expand it will cause the outer material to stretch in these directions. Inside the rectangle the material is compressed in the  $\tilde{x}_1$  and  $\tilde{x}_2$  direction. This is expected as the outer material is trying to compress the inner material. The behaviour in the  $\tilde{x}_3$  direction of the inner material is a little harder to understand. Away from the interface we see that the material is compressed in the  $\tilde{x}_3$  direction

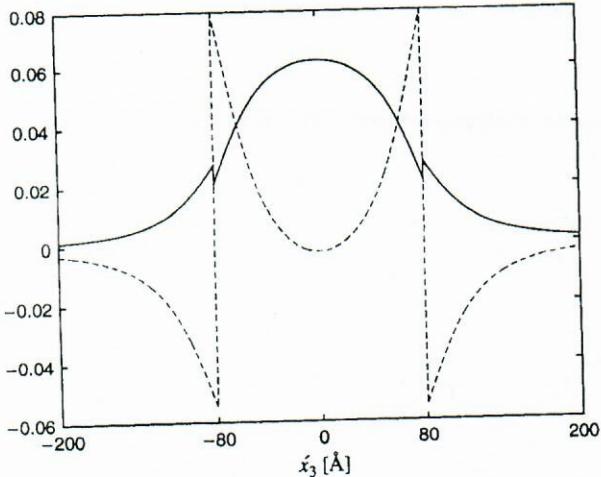


Fig. 8. Strain components with respect to the reference configuration for a rectangular inclusion in the  $x_3$ -direction with  $x_1 = 0$  and  $x_2 = 0$  for a structure where  $a = b = 40$  and  $c = 80$ . The solid line is  $\epsilon_{11} = \epsilon_{22}$  and the dashed line is  $\epsilon_{33}$ .

Table II. The ground state energies  $E_g$  and first excited state energies  $E_1$  for a rectangular inclusion of InAs in GaAs.

	No strain	Strain to first-order	Strain to second order
$E_g$	0.234 eV	0.696 eV	0.668 eV
$E_1$	0.337 eV	0.775 eV	0.750 eV

as expected, however, close to the interface it is actually stretched. This is surprising because it is expected that the whole material would be compressed. This behaviour can be understood in the following way. When a material is compressed in one direction it will usually expand in the perpendicular directions. So, if the inner material is free to move in the  $\tilde{x}_3$  direction the material would be stretched. What happens in the case where the inner material is blocked by the outer material is that the tendency of the inner material to stretch wins over the tendency of the outer material to compress the inner material, at least close to the interface.

In Figure 8 the strain profile relative to the reference configuration ( $\epsilon$ ) is shown along the  $x_3$  axis ( $x_1 = x_2 = 0$ ). The main difference is that the strain in the inner material is no longer negative but instead positive.

### 2.2.1. Electronic Band-Structure

The strain one band model derived in section 1.2 has been implemented using a finite element method for the rectangular quantum dot and the resulting ground state and first excited state energies with respect to a model without strain, a model using the first-order approximation and a model using the second-order approximation are listed in Table II.

The material parameters used are taken from Vurgaftman et al.<sup>9</sup> and they are given in Table III.

The error in not taking strain into account relative to the second-order result is seen to be 65 % for the ground state and 45 % for the first excited state and the error in using the first-order approximation relative to the second-order results is 4 % for the ground state and 3.3 % for the first excited state. It is seen that it is quite important to include strain in the calculation of the energy band-structure for this system and that the second-order contributions are by no means negligible. Whether or not third or higher-order terms are negligible has to be verified by including these terms in the Taylor series expansion, however, as long as the strain  $\epsilon$  is not higher than 8%, which is the case here, third or higher-order terms will be in the order of  $\epsilon^3$  or less. In situations with larger strain the higher-order terms will become increasingly important.

Table III. Material parameters for InAs and GaAs.

	$m_c [m_e]$	$E_c$ [eV]	$a_c$ [eV]
InAs	0.026	0	-5.08
GaAs	0.067	0.892	-7.17

### 3. CONCLUSION

In this paper a general method for treating Hamiltonians of deformed nanoscale systems based on a Taylor series expansion has been employed to find second-order approximations with respect to a known deformation both within a weak and a strong formulation of the problem. The weak formulation of the problem was needed in order to allow the deformation gradient to have discontinuities at interfaces. In the case of the strong formulation of the problem appropriate interface boundary conditions were derived directly from the weak formulation of the problem. Also, a second-order approximation with respect to a known strain tensor was derived. This was needed as the strain tensor is usually easier to find than the deformation itself. As an example, the electronic energies of a one-dimensional strained Kronig-Penney potential were presented for an exact, a first-order and a second-order strain Hamiltonians. In addition, the example of a rectangular quantum dot was studied, where the strain tensor was found based on linear isotropic strain theory. Our results show that the second-order strain Hamiltonian can be applied to the band-structure analysis with the Kronig-Penney model at least for a maximum strain of up to 18% giving an error of less than 1%. In the quantum dot

example, it was seen that the inclusion of strain in the Hamiltonian is of paramount importance for InAs/GaAs structures. Here it was seen that the error in disregarding strain effects relative to the second-order approximation was 65% for the ground-state. It was also seen that second-order contributions are not negligible.

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