A general treatment of deformation effects in Hamiltonians for nanoscale systems

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Abstract

In this paper a general method of treating Hamiltonians of deformed nanoscale systems is proposed. This method is used to derive a second-order strain Hamiltonian. As an example, energies for a one-dimensional strained Krönig–Penney potential are calculated with exact, first-order, and second-order strain Hamiltonians.

Keywords: Deformations; Nonlinear strain effects; Quantum mechanics; Crystal Hamiltonian; Krönig–Penney model; Taylor series expansion

1. Introduction

Nanoscale semiconductor devices usually consist of materials with different lattice constants, hence these structures will be strained. It is known that strain strongly affects the electronic and optical properties, hence in order to be able to model these devices it is important to account for strain effects. It is well known how to incorporate homogeneous strain in electronic bandstructure calculations [1], but in nanoscale hetero-structures strain is no longer homogeneous. Zhang [2] and Suzuki [3] have proposed two different methods to include linear inhomogeneous strain terms in the Hamiltonian under certain assumptions for the strain and the potential. In this paper, a general method of treating Hamiltonians of deformed nanoscale systems (e.g. an inhomogeneous strained Hamiltonian) is proposed based on a Taylor series expansion. The methodology is explained on the example of the Krönig–Penney model, and the results of the analysis of this model with a higher-order Hamiltonian are compared with those previously reported in the literature.

2. Theory

A deformation $\phi: \mathcal{B} \to \mathbb{R}^3$ of an underformed domain $\mathcal{B}$, e.g. a crystal volume, is a C^2 map satisfying $\inf(\det(\nabla\phi)) \neq 0$. It is assumed throughout this paper

that $\mathcal{B}$ is compact. This ensures boundness of considered operators, the derivatives of the deformation, and the derivative of the inverse of the deformation. The space of all deformations of $\mathcal{B}$ is denoted $\mathcal{D}$, primed ($'$) coordinates, functions, and operators always refer to the domain $\mathcal{B}$, while unprimed coordinates, functions, and operators refer to the domain $\phi(\mathcal{B})$ (see Fig. 1).

An electron in a potential deformed by ϕ is subject to the potential $V(F)$, where F signifies that the potential depends only on ϕ through the deformation gradient $F = \nabla'\phi$. The Hamiltonian of the deformed system, referred to as the deformed Hamiltonian, is then given by:

$$H_F = -\frac{\hbar^2}{2m}\Delta + V(F) \qquad (1)$$

In what follows we assume that the domain of the deformed Hamiltonian is the Sobolev space $W^{2,2}(\phi(\mathcal{B}))$. In this way possible potentials also encompass distributions such as the Dirac-delta function (see Section 3).

From the inverse function theorem it follows that ϕ has a C^2 inverse defined on $\phi(\mathcal{B})$. This ensures that $H_{\nabla'\phi}$ can be written with respect to coordinates on $\mathcal{B}$. As a result, the deformed Hamiltonian can be viewed as an operator

$$\hat{H}: \mathcal{D} \to L(W^{2,2}(\mathcal{B}), L^2(\mathcal{B})) \qquad (2)$$

given by $\phi \to H_{\nabla'\phi}$, where $L(\mathcal{F}, \mathcal{G})$ is the space of bounded linear mappings from $\mathcal{F}$ to $\mathcal{G}$ and $L^2(\mathcal{B})$ is the

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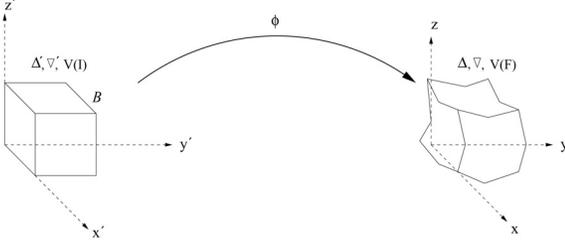
Fig. 1. A sketch of a deformation with related operators and functions used.

Lebesgue space. The space $\mathcal{D}$ is equipped with the supremum norm, $W^{2,2}(\mathcal{B})$ is equipped with the corresponding Sobolev norm, and $L(W^{2,2}(\mathcal{B}), L^2(\mathcal{B}))$ is equipped with the operator norm (e.g. [4,5]).

Since the undeformed potential is usually better known than the deformed potential and the deformation is known, it is more convenient to express the Hamiltonian in terms of these quantities. The easiest way to do that is to make a Taylor series expansion of $\hat{H}$ around the identity function on $\mathcal{B}$ denoted *id*. By noting that the deformed Hamiltonian depends only on ϕ through F, it is found that the deformed Hamiltonian is to the second-order in F given by

$$H_F \approx H_I + D_F^{(1)} \cdot (F - I) + D_F^{(2)} \cdot (F - I, F - I) \qquad (3)$$

where

$$H_I = -\frac{\hbar^2}{2m}\Delta' + V(I) \qquad (4)$$

$$D_F^{(1)} \cdot (F - I) = \frac{\hbar^2}{2m}\left\{ \sum_{j=1}^{3}\sum_{k=1}^{3}[F + F^T - 2I]_{jk}\frac{\partial}{\partial x'_j}\frac{\partial}{\partial x'_k} + \right.$$

$$\left. \sum_{i=1}^{3}\sum_{k=1}^{3}\frac{\partial}{\partial x'_i}([F - I]_{ki})\frac{\partial}{\partial x'_k}\right\} + DV(I) \cdot (F - I) \qquad (5)$$

$$D_F^{(2)} \cdot (F - I, F - I) = -\frac{\hbar^2}{2m}\left\{ \sum_{j=1}^{3}\sum_{k=1}^{3}[(F - I)(F - I)^T]_{jk} \right.$$

$$\frac{\partial}{\partial x'_j}\frac{\partial}{\partial x'_k} + \sum_{i=1}^{3}\sum_{j=1}^{3}\sum_{k=1}^{3}[(F - I)]_{ji}\frac{\partial}{\partial x'_j}([F - I]_{ki})\frac{\partial}{\partial x'_k} +$$

$$\sum_{j=1}^{3}\sum_{k=1}^{3}[(F - I)^2 + (F^T - I)^2]_{jk}\frac{\partial}{\partial x'_j}\frac{\partial}{\partial x'_k} + \sum_{i=1}^{3}\sum_{k=1}^{3}$$

$$\frac{\partial}{\partial x'_i}[(F - I)^2]_{ki}\frac{\partial}{\partial x'_k}\right\} + \frac{1}{2}D^2V(I) \cdot ((F - I), (F - I))$$

$$(6)$$

where $I = \nabla' id$. The notations used are identical to those in Marsden et al. [6]. This Hamiltonian is referred to as the second-order strain Hamiltonian. The error introduced by this approximation is known to be of the third order in $(F - I)$ (see, e.g. [7]).

The detailed derivation of this expression and the inclusion of spin in the Hamiltonian is outside the scope of this short communication and will be presented in a forthcoming article. Under the assumption that the deformation gradient F is symmetric and employing the linear strain tensor, the first order Taylor expansion is identical to the strain Hamiltonian derived by Zhang [2] disregarding spin.

3. Strained Krönig–Penney potential

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

$$V(I)(x') = \frac{3\pi\hbar^2}{2ma}\sum_{n=-N}^{N}\delta(x' - na) \qquad (7)$$

for $x' \in [-Na, Na] = \mathcal{B}$, where $N \in \{\mathbb{N}\ a \in\ ]0, \infty[$ is the lattice constant, and δ is the Diracdelta function. In addition to this, periodic boundary conditions are imposed. Figure 2 shows the first three energy bands obtained. Assuming that $N/10 \in \mathbb{N}$, a strained Krönig–Penney potential is found by deforming the above potential by $\phi(x') = x' + \varepsilon a \sin(2\pi x'/10a)$
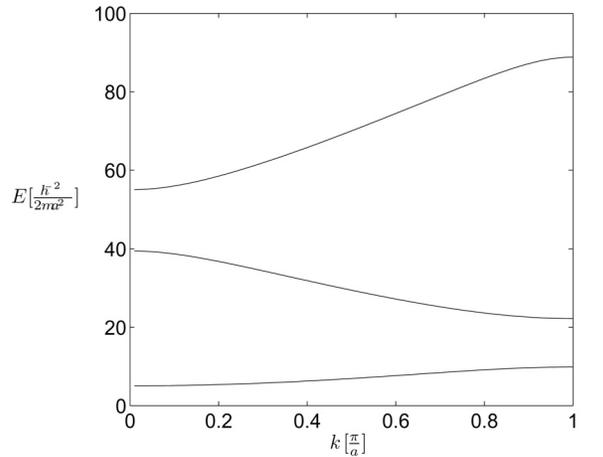
Fig. 2. Energy bands for the unstrained Krönig–Penney potential.

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

$$H_F = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{3\pi\hbar^2}{2ma}\sum_{n=-N}^{N}\delta(x - \phi(na)) \qquad (8)$$

The problem of finding the energy eigenvalues and associated eigenfunctions of this Hamiltonian is straight-forward and it reduces to the problem of solving a nonlinear equation.

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. (8) it is found that

$$V(F)(x') = \frac{3\pi\hbar^2}{2ma} \sum_{n=-N}^{N} \delta(\phi x') - \phi(na)) = \frac{3\pi\hbar^2}{2ma} \sum_{n=-N}^{N}$$

$$\frac{\delta(x' - na)}{F(na)} \qquad (9)$$

where $F(x'_0) = \partial\phi/\partial x'\big|_{x'_0} = 1 + 2\pi\epsilon/10 \cos(2\pi x'_0/10a)$. Notice that in this example F is always positive. The second-order strain Hamiltonian is then given by

$$\begin{aligned}
H_F &\approx \frac{\hbar^2}{2m}\left(-1 + 2(F-1) - 3(F-1)^2\right)\frac{\partial^2}{\partial x'^2} \\
&+ \frac{\hbar^2}{2m}\left(\frac{\partial(F-1)}{\partial x'} - (F-1)\frac{\partial(F-1)}{\partial x'} - \frac{\partial(F-1)^2}{\partial x'}\right)\frac{\partial}{\partial x'} \\
&+ \frac{3\pi\hbar^2}{2ma}\sum_{n=-N}^{N}\left(\delta(x'-na)\left(1 - (F-1) + (F-1)^2\right)\right) \quad (10)
\end{aligned}$$

The solutions to the eigenvalue equation for this Hamiltonian were found using the finite element method. In Fig. 3 results are shown for the unstrained, strained exact, strained first-order, and strained second-order Taylor expansions for $\epsilon = 0.2$. 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 were made for different ϵ values at the zone center. In Fig. 4 the difference between the energy of the first state calculated with the exact Hamiltonian and the first-order and second-order approximations is shown as a function of ϵ and the maximal Green-Lagrange-St. Venant strain. The errors of the first and the second-order Hamiltonians are given by

$$\text{Error}^{\text{x}} = \left|\frac{E_1^{\text{Exact}} - E_1^{\text{x}}}{E_1^{\text{Exact}}}\right|, \text{ x = 1st, 2nd} \qquad (11)$$

where E_1^{Exact}, E_1^{1st} and E_1^{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

$$\mathcal{E}(x'_0) = \frac{1}{2}\left(F(x'_0)^T F(x'_0) - I\right) = \frac{2\pi\varepsilon}{10}\cos\left(\frac{2\pi}{10a}x'_0\right)$$

$$\left(1 + \frac{\pi\varepsilon}{10}\cos\left(\frac{2\pi}{10a}x'_0\right)\right) \qquad (12)$$

i.e. the maximal strain is given by $\frac{2\pi\varepsilon}{10}\left(1 + \frac{\pi\varepsilon}{10}\right)$.

From Fig. 4 it can be seen that both the first-order and second-order approximations are quite accurate up to a max strain of 7% as the error is less than 1%. It is of particular interest to note that the second-order approximation has an error of less than 1% for
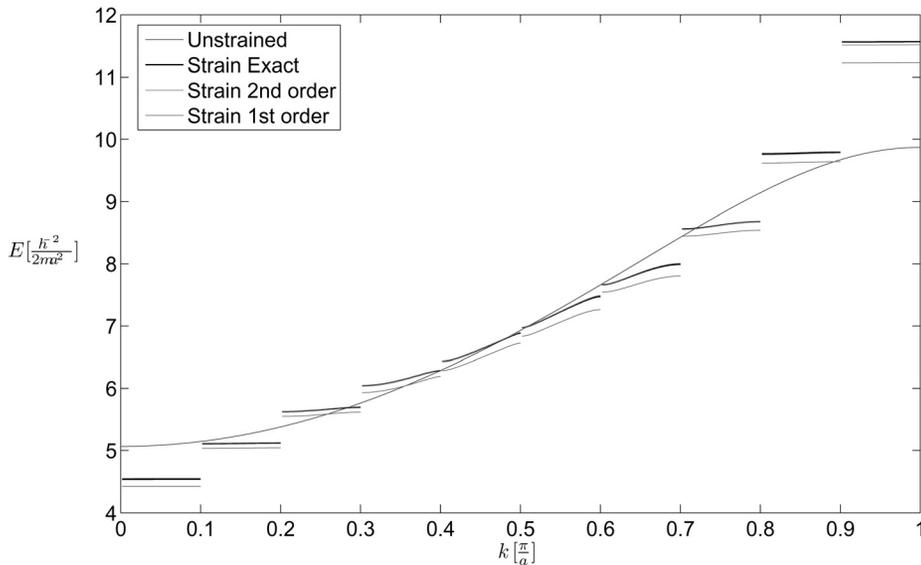
Fig. 3. Energy bands for the strained Krönig–Penney potential for $\epsilon = 0.2$.
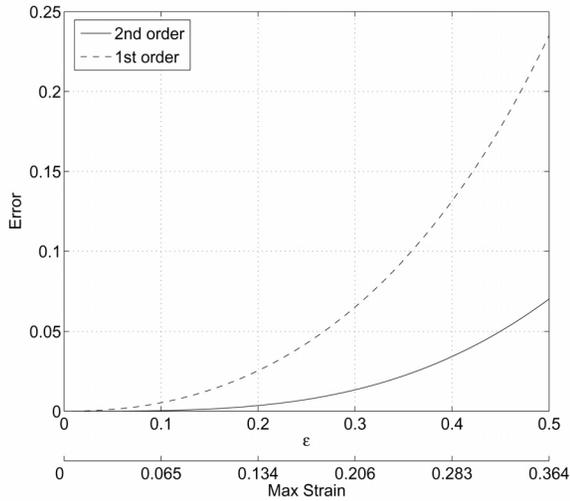
Fig. 4. Error of the first-order and second-order strained Hamiltonian at the zone center.

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.

4. Conclusion

In this paper a general method for treating Hamiltonians of deformed nanoscale systems has been proposed based on a Taylor series expansion. This method was employed to find the second-order strain Hamiltonian. As an example, the electronic energies of a one-dimensional strained Krönig–Penney potential were presented for exact, first-order, and second-order strain Hamiltonians. Our results show that the second-order strain Hamiltonian can be applied to the band structure analysis with the Krönig–Penney model at least for a maximum strain of up to 18% giving an error of less than 1%.

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