# Hamiltonians of strain effects

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Hamiltonians that generally describe the effects of strain are proposed. The strain effects can be calculated easily from the unstrained potential using these Hamiltonians. These Hamiltonians are valid when the strain is spatially modulated, and are also valid when the strain exists in a magnetic field. These Hamiltonians can also be used in the improved effective mass approximation.

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Semiconductor strain structures are made from materials with different lattice constants. Recently attempts to use strain structures as the low-dimensional quantum confinements such as quantum wells, quantum wires, or quantum dots have become popular. Self-assembled quantum dots grown in the Stranski-Krastanow mode[1] are using the strain confinements. GaN-type semiconductor blue lasers stimulated by current injection use the strain structures as the active layers.[2] *Spin devices* that use magnetic nanostructures[3] are always associated with strain fields. And the magnetoresistance oscillation of two-dimensional electron gas under one-dimensional periodic potential modulation includes the strain-induced component,[4] whose amplitude cannot be estimated from the theory.

Davies *et al.*[5] proposed the theories of the confinement potential in the quantum strain structures. Their theories are based on the classical mechanics of elastic body and the classical electromagnetism, so the results do not include the quantum effects, for example, the effect of the charge-density wave.

The electronic states in the quantum strain structures are calculated from the first principle, if the systems are simple. But the electronic states in the complicated strain structures cannot be calculated from the first principle because of the limited ability of computers.

The effect of strain was formulated by Pikus and Bir,[6,7] and it is known as *the Pikus-Bir Hamiltonian*. However, the Pikus-Bir Hamiltonian is valid only when the strain is homogeneous. It is invalid when the strain is spatially modulated in the low-dimensional quantum structures, and moreover it is invalid when the strain exists in a magnetic field. Hence in this paper I propose Hamiltonians that generally describe the effects of strain.

Strain means that a point in an object shifts from a position $\boldsymbol{x}$ to a position $\boldsymbol{x}'$. Here, displacement $\boldsymbol{u}(\boldsymbol{x})$ is defined as a function of the position $\boldsymbol{x}$,

$$\boldsymbol{x}' = \boldsymbol{x} + \boldsymbol{u}(\boldsymbol{x}). \tag{1}$$

First we consider the case $\boldsymbol{u}(\boldsymbol{x}) = \boldsymbol{a}$, which is not a function of the position but a real constant vector. In this case the strain becomes a mere parallel translation. The transformation of an observable $\mathcal{A}$ in a parallel translation is well known in quantum mechanics.[8] The transformation is expressed by a unitary operator $T(\boldsymbol{a})$ as follows:

$$\mathcal{A} \rightarrow T(\boldsymbol{a})\mathcal{A}T^{\dagger}(\boldsymbol{a}), \tag{2}$$

$$T(\boldsymbol{a}) = e^{-i\boldsymbol{a}\cdot\boldsymbol{p}/\hbar}, \tag{3}$$

where $\boldsymbol{p}$ is a momentum operator $[\boldsymbol{p} = (\hbar/i)\nabla]$.

Next, we consider the general case that the displacement $\boldsymbol{u}(\boldsymbol{x})$ is a function of the position $\boldsymbol{x}$. In this case we cannot define a transformation operator $T[\boldsymbol{u}(\boldsymbol{x})] = \exp[-i\boldsymbol{u}(\boldsymbol{x})\cdot\boldsymbol{p}/\hbar]$ to replace simply the real constant vector $\boldsymbol{a}$ with the displacement $\boldsymbol{u}(\boldsymbol{x})$. The reason is that the operator $T[\boldsymbol{u}(\boldsymbol{x})]$ is not a unitary operator anymore, because the displacement $\boldsymbol{u}(\boldsymbol{x})$ is a function of the position $\boldsymbol{x}$ and does not commute with the momentum $\boldsymbol{p}$. A transformation operator must be a unitary operator in order to guarantee an observable to be a Hermitian operator.

Hence when the displacement $\boldsymbol{u}(\boldsymbol{x})$ is small, I propose a transformation operator $\mathcal{T}[\boldsymbol{u}(\boldsymbol{x})]$ that describes a strain effect,

$$\mathcal{A} \rightarrow \mathcal{T}[\boldsymbol{u}(\boldsymbol{x})]\mathcal{A}\mathcal{T}^{\dagger}[\boldsymbol{u}(\boldsymbol{x})], \tag{4}$$

$$\mathcal{T}[\boldsymbol{u}(\boldsymbol{x})] = \exp\{-i[\boldsymbol{u}(\boldsymbol{x})\cdot\boldsymbol{p} + \boldsymbol{p}\cdot\boldsymbol{u}(\boldsymbol{x})]/2\hbar\}. \tag{5}$$

The transformation operator $\mathcal{T}[\boldsymbol{u}(\boldsymbol{x})]$ becomes a unitary operator because the term $[\boldsymbol{u}(\boldsymbol{x})\cdot\boldsymbol{p} + \boldsymbol{p}\cdot\boldsymbol{u}(\boldsymbol{x})]/2$ in the exponential function of the transformation operator is *Hermitization of the operator*.[9] Thus,

$$\begin{aligned}\mathcal{T}[\boldsymbol{u}(\boldsymbol{x})]&\mathcal{A}\mathcal{T}^{\dagger}[\boldsymbol{u}(\boldsymbol{x})] \\ &= \exp\{-i[\boldsymbol{u}(\boldsymbol{x})\cdot\boldsymbol{p} + \boldsymbol{p}\cdot\boldsymbol{u}(\boldsymbol{x})]/2\hbar\}\mathcal{A}\exp\{i[\boldsymbol{u}(\boldsymbol{x})\cdot\boldsymbol{p} \\ &\quad + \boldsymbol{p}\cdot\boldsymbol{u}(\boldsymbol{x})]/2\hbar\} \qquad (6)\\ &\approx \mathcal{A} + \frac{i}{2\hbar}[\mathcal{A}, \boldsymbol{u}(\boldsymbol{x})\cdot\boldsymbol{p} + \boldsymbol{p}\cdot\boldsymbol{u}(\boldsymbol{x})] \qquad (7)\\ &= \mathcal{A} + \frac{1}{2}\left[\mathcal{A}, u_j\frac{\partial}{\partial x_j} + \frac{\partial}{\partial x_j}u_j\right] \quad (j = 1,2,3). \qquad (8)\end{aligned}$$

From Eq. (6) to Eq. (7) the next relationship is used, and the terms are adopted up to the first order about the displacement $\boldsymbol{u}(\boldsymbol{x})$ because $\boldsymbol{u}(\boldsymbol{x})$ is small enough,

$$e^{-B}A\,e^{B} = A + [A,B] + \tfrac{1}{2}[[A,B],B] + \cdots. \tag{9}$$

In the component expression of Eq. (8), we use Einstein's summation convention about the same appendixes.

 

Now we consider the Hamiltonians that describe the effects of strain using the transformation operator $\mathcal{T}$. The Schrödinger equation for an electron in a strained crystal is

$$\mathcal{H}_\varepsilon \psi_\varepsilon = (\mathcal{K} + V_\varepsilon)\psi_\varepsilon = E_\varepsilon \psi_\varepsilon , \tag{10}$$

where $\mathcal{H}_\varepsilon$ is a Hamiltonian of the strained crystal, which includes the kinetic energy term $\mathcal{K}$ and the unknown strained potential $V_\varepsilon$. We want to calculate the energies $E_\varepsilon$ and the wave functions $\psi_\varepsilon$. The Schrödinger equation of the unstrained crystal is

$$\mathcal{H}\psi = (\mathcal{K} + V)\psi = E\psi, \tag{11}$$

where $V$ is the unstrained potential. Here we note that we cannot interpret the difference $V_\varepsilon - V$ directly as a perturbation, since it is generally not small.[7] For example, in the case of a Coulomb potential generated by an atomic nucleus, the difference $V_\varepsilon - V$ becomes infinite, however small the displacement $\boldsymbol{u}(\boldsymbol{x})$ is. Therefore I propose a Hamiltonian $\tilde{\mathcal{H}} = \mathcal{T}^\dagger \mathcal{K} \mathcal{T} + V$ that describes the strain effect to replace the difference of the potentials with the change of the kinetic energy term,

$$\tilde{\mathcal{H}}\phi = (\mathcal{T}^\dagger \mathcal{K} \mathcal{T} + V)\phi = \mathcal{E}\phi. \tag{12}$$

$\mathcal{T}$ is operated from the left, and $\mathcal{T}^\dagger \mathcal{T} = 1$ is inserted,

$$\mathcal{T}(\mathcal{T}^\dagger \mathcal{K} \mathcal{T} + V)(\mathcal{T}^\dagger \mathcal{T})\phi = \mathcal{E}\mathcal{T}\phi, \tag{13}$$

$$(\mathcal{K} + \mathcal{T}V\mathcal{T}^\dagger)(\mathcal{T}\phi) = \mathcal{E}(\mathcal{T}\phi). \tag{14}$$

Regarding $\mathcal{T}V\mathcal{T}^\dagger \approx V_\varepsilon$,

$$(\mathcal{K} + V_\varepsilon)(\mathcal{T}\phi) = \mathcal{E}(\mathcal{T}\phi). \tag{15}$$

Comparing Eq. (15) with Eq. (10), $E_\varepsilon \approx \mathcal{E}$ and $\psi_\varepsilon \approx \mathcal{T}\phi$. After all, by solving Eq. (12) that uses the unstrained potential $V$, the electronic states in the strained crystal can be calculated.

In the first problem, we transform a Hamiltonian $\mathcal{H}_{\mathrm{zero}}$ in a zero magnetic field,

$$\mathcal{H}_{\mathrm{zero}} = -\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{ex}}(\boldsymbol{x}) + V_{\mathrm{st}}(\boldsymbol{x}) \tag{16}$$

$$= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_i \partial x_i} + V_{\mathrm{ex}} + V_{\mathrm{st}} \quad (i = 1,2,3). \tag{17}$$

Here we must pay attention to two kinds of potential, $V_{\mathrm{ex}}(\boldsymbol{x})$ and $V_{\mathrm{st}}(\boldsymbol{x})$. $V_{\mathrm{ex}}(\boldsymbol{x})$ is an external field, which is independent of a strain. That is to say, the magnitude of $V_{\mathrm{ex}}(\boldsymbol{x})$ does not change even if a strain exists. In contrast, the magnitude of $V_{\mathrm{st}}(\boldsymbol{x})$ changes as a strain changes. For example, $V_{\mathrm{st}}(\boldsymbol{x})$ is a potential that is generated by atomic nuclei and bound electrons in a strained object. In the transformation, we regard $V_{\mathrm{st}}(\boldsymbol{x})$ as not a function of the position $\boldsymbol{x}$ but a real constant scalar. Thus,

$$\widetilde{\mathcal{H}_{\mathrm{zero}}} = \mathcal{T}^\dagger \left( -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_i \partial x_i} + V_{\mathrm{ex}} \right)\mathcal{T} + V_{\mathrm{st}} \tag{18}$$

$$\approx -\frac{\hbar^2}{2m}\left( \frac{\partial^2}{\partial x_i \partial x_i} - 2\frac{\partial u_j}{\partial x_i}\frac{\partial^2}{\partial x_i \partial x_j} - \frac{\partial^2 u_j}{\partial x_i \partial x_i}\frac{\partial}{\partial x_j} - \frac{\partial^2 u_j}{\partial x_i \partial x_j} \times \frac{\partial}{\partial x_i} - \frac{1}{2}\frac{\partial^3 u_j}{\partial x_i \partial x_i \partial x_j} \right) + \left( V_{\mathrm{ex}} + u_j \frac{\partial V_{\mathrm{ex}}}{\partial x_j} \right) + V_{\mathrm{st}} \tag{19}$$

$$= -\frac{\hbar^2}{2m}\left( \frac{\partial^2}{\partial x_i \partial x_i} - 2\varepsilon_{ij}\frac{\partial^2}{\partial x_i \partial x_j} - \frac{\partial \varepsilon_{ij}}{\partial x_i}\frac{\partial}{\partial x_j} - \frac{\partial \varepsilon_{ij}}{\partial x_j}\frac{\partial}{\partial x_i} - \frac{1}{2}\frac{\partial^2 \varepsilon_{ij}}{\partial x_i \partial x_j} \right) + \left( V_{\mathrm{ex}} + u_j \frac{\partial V_{\mathrm{ex}}}{\partial x_j} \right) + V_{\mathrm{st}}. \tag{20}$$

We note that the differential of the third order about the displacement $\boldsymbol{u}(\boldsymbol{x})$ appears in Eq. (19). The change of $V_{\mathrm{ex}}(\boldsymbol{x})$ in Eq. (20) cannot be expressed by the strain tensor $\varepsilon_{ij} \equiv (\partial u_i/\partial x_j + \partial u_j/\partial x_i)/2$. If the strain is homogeneous $(\partial \varepsilon_{ij}/\partial x_k = 0)$, Eq. (20) becomes the Pikus-Bir Hamiltonian.

In the second problem, we transform a Hamiltonian $\mathcal{H}_{\mathrm{mag}}$ in a magnetic field,

$$\mathcal{H}_{\mathrm{mag}} = \frac{1}{2m}\left\{ \frac{\hbar}{i}\nabla - e[\boldsymbol{A}_{\mathrm{ex}}(\boldsymbol{x}) + \boldsymbol{A}_{\mathrm{st}}(\boldsymbol{x})] \right\}^2 + V_{\mathrm{ex}}(\boldsymbol{x}) + V_{\mathrm{st}}(\boldsymbol{x}) \tag{21}$$

$$= \mathcal{H}_{\mathrm{zero}} + \frac{1}{2m}\left\{ -\frac{e\hbar}{i}\left[ 2(A_{\mathrm{ex},i} + A_{\mathrm{st},i})\frac{\partial}{\partial x_i} + \frac{\partial (A_{\mathrm{ex},i} + A_{\mathrm{st},i})}{\partial x_i} \right] + e^2 (A_{\mathrm{ex},i} + A_{\mathrm{st},i}) \times (A_{\mathrm{ex},i} + A_{\mathrm{st},i}) \right\}. \tag{22}$$

We must pay attention to two kinds of vector potential $\boldsymbol{A}_{\mathrm{ex}}(\boldsymbol{x})$ and $\boldsymbol{A}_{\mathrm{st}}(\boldsymbol{x})$ also. $\boldsymbol{A}_{\mathrm{ex}}(\boldsymbol{x})$ is an external magnetic field, which is independent of a strain. In contrast, the magnitude of $\boldsymbol{A}_{\mathrm{st}}(\boldsymbol{x})$ changes as a strain changes. For example, $\boldsymbol{A}_{\mathrm{st}}(\boldsymbol{x})$ is generated by the magnetic substances buried in a strained object. Note that from Eq. (21) to Eq. (22), both $\boldsymbol{A}_{\mathrm{ex}}(\boldsymbol{x})$ and $\boldsymbol{A}_{\mathrm{st}}(\boldsymbol{x})$ are transformed as functions of the position $\boldsymbol{x}$. However, from Eq. (22) to Eq. (23), $\boldsymbol{A}_{\mathrm{ex}}(\boldsymbol{x})$ is transformed as a function of the position $\boldsymbol{x}$, while $\boldsymbol{A}_{\mathrm{st}}(\boldsymbol{x})$ is transformed as a real constant vector. Thus,

$$\widetilde{\mathcal{H}_{\mathrm{mag}}} \approx \widetilde{\mathcal{H}_{\mathrm{zero}}} + \frac{1}{2m}\left\{ -\frac{e\hbar}{i}\left[ 2(A_{\mathrm{ex},i} + A_{\mathrm{st},i})\frac{\partial}{\partial x_i} + \frac{\partial (A_{\mathrm{ex},i} + A_{\mathrm{st},i})}{\partial x_i} - 2(A_{\mathrm{ex},i} + A_{\mathrm{st},i})\frac{\partial u_j}{\partial x_i}\frac{\partial}{\partial x_j} + 2u_j \frac{\partial A_{\mathrm{ex},i}}{\partial x_j}\frac{\partial}{\partial x_i} - (A_{\mathrm{ex},i} + A_{\mathrm{st},i})\frac{\partial^2 u_j}{\partial x_i \partial x_j} + u_j \frac{\partial^2 A_{\mathrm{ex},i}}{\partial x_i \partial x_j} \right] + e^2 \left[ (A_{\mathrm{ex},i} + A_{\mathrm{st},i})(A_{\mathrm{ex},i} + A_{\mathrm{st},i}) + 2u_j (A_{\mathrm{ex},i} + A_{\mathrm{st},i})\frac{\partial A_{\mathrm{ex},i}}{\partial x_j} \right] \right\}. \tag{23}$$

If a vector potential exists, the Hamiltonian of a strain effect cannot be expressed as a function of the strain tensor $\varepsilon_{ij}$ any longer because the Hamiltonian of a strain effect includes the displacement $\boldsymbol{u}(\boldsymbol{x})$ obviously.

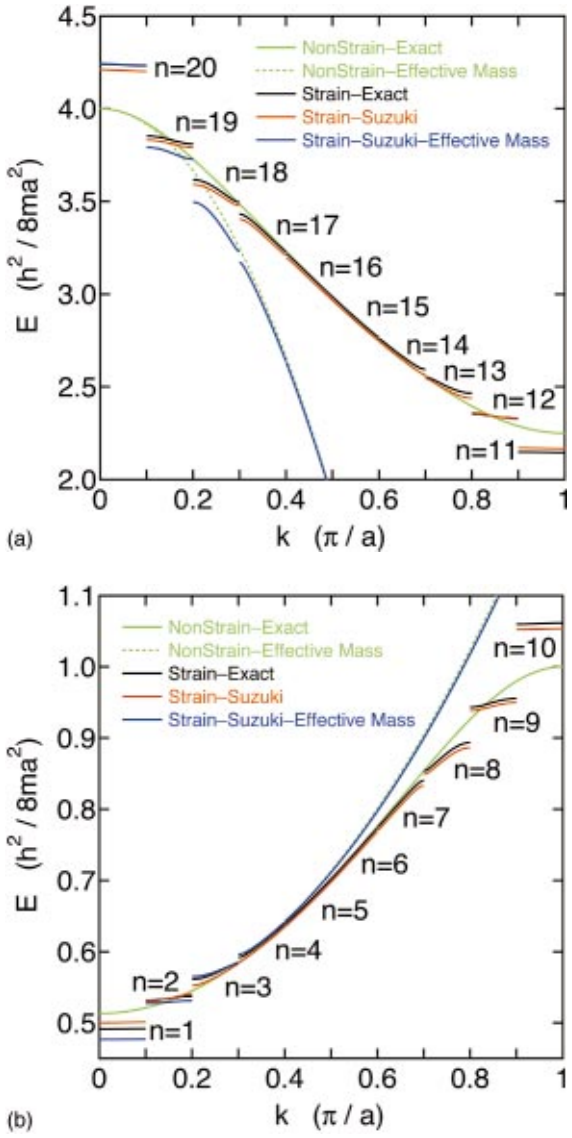


FIG. 1. (Color) Energy dispersions of a one-dimensional strained Kronig-Penney model in a zero magnetic field.

Now I derive the Hamiltonian of a strain effect in the improved effective mass approximation following Luttinger and Kohn.[10] $\tilde{\mathcal{H}}$ in Eq. (12) is divided into the unstrained Hamiltonian $\mathcal{H}$ and the perturbation term $\mathcal{H}_1$,

$$\tilde{\mathcal{H}}=\mathcal{H}+(\tilde{\mathcal{H}}-\mathcal{H})\equiv\mathcal{H}+\mathcal{H}_1. \tag{24}$$

The wave function $\phi\approx\Sigma_{\boldsymbol{k}}C_{\boldsymbol{k}}\psi_{\boldsymbol{k}}$, which is expanded by the unstrained wave functions in the same band,

$$(\mathcal{H}+\mathcal{H}_1)\sum_{\boldsymbol{k}} C_{\boldsymbol{k}}\psi_{\boldsymbol{k}}=\mathcal{E}\sum_{\boldsymbol{k}} C_{\boldsymbol{k}}\psi_{\boldsymbol{k}}. \tag{25}$$

Multiplied by $\psi^*_{\boldsymbol{k}'}$ from the left and integrated,

$$[E(\boldsymbol{k}')-\mathcal{E}]C_{\boldsymbol{k}'}+\sum_{\boldsymbol{k}}\langle\boldsymbol{k}'|\mathcal{H}_1|\boldsymbol{k}\rangle C_{\boldsymbol{k}}=0. \tag{26}$$

Multiplied by $e^{i\boldsymbol{k}'\cdot\boldsymbol{x}}$ and added over $\boldsymbol{k}'$,

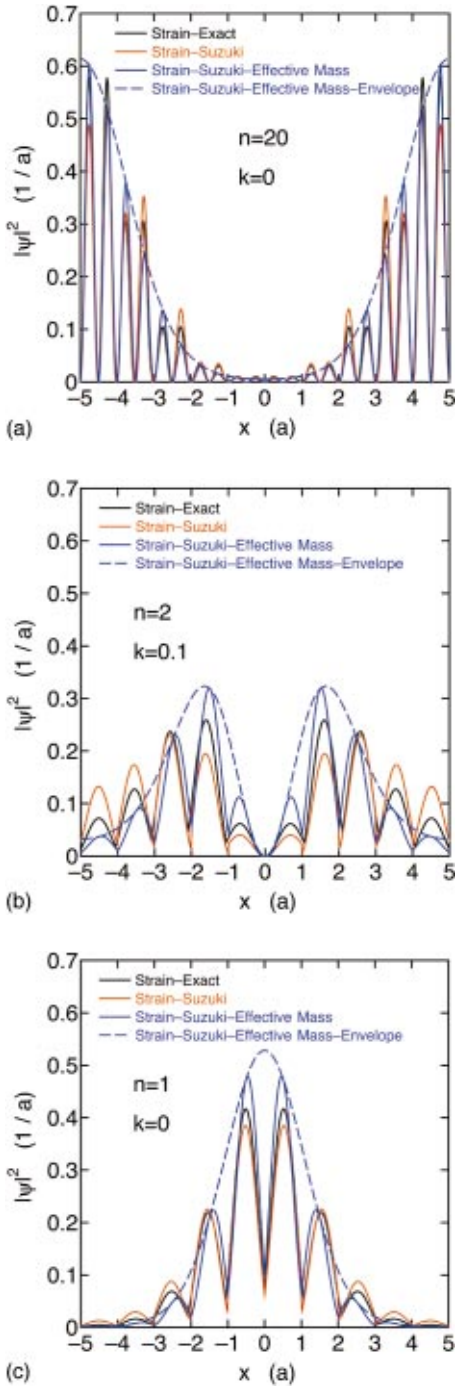


FIG. 2. (Color) Wave functions of a one-dimensional strained Kronig-Penney model in a zero magnetic field.

$$\sum_{k'}[E(\boldsymbol{k}')-\mathcal{E}]C_{\boldsymbol{k}'}e^{i\boldsymbol{k}'\cdot\boldsymbol{x}}+\sum_{\boldsymbol{k},\boldsymbol{k}'}\langle\boldsymbol{k}'|\mathcal{H}_1|\boldsymbol{k}\rangle C_{\boldsymbol{k}}e^{i\boldsymbol{k}'\cdot\boldsymbol{x}}=0. \tag{27}$$

The envelope function $F=\Sigma_{\boldsymbol{k}}C_{\boldsymbol{k}}e^{i\boldsymbol{k}\cdot\boldsymbol{x}}$ is defined,

$$[E(-i\nabla)-\mathcal{E}]F+\sum_{\boldsymbol{k},\boldsymbol{k}'}\langle\boldsymbol{k}'|\mathcal{H}_1|\boldsymbol{k}\rangle C_{\boldsymbol{k}}e^{i\boldsymbol{k}'\cdot\boldsymbol{x}}=0. \tag{28}$$

The second term in Eq. (19) is used as an example of $\mathcal{H}_1$,

$$\sum_{\boldsymbol{k},\boldsymbol{k}'} \langle \boldsymbol{k}'|\mathcal{H}_1|\boldsymbol{k}\rangle C_{\boldsymbol{k}} e^{i\boldsymbol{k}'\cdot\boldsymbol{x}}$$

$$= \sum_{\boldsymbol{k},\boldsymbol{k}'} C_{\boldsymbol{k}} e^{i\boldsymbol{k}'\cdot\boldsymbol{x}} \int \psi^*_{\boldsymbol{k}'} \frac{\hbar^2}{m} \frac{\partial u_j}{\partial x_i} \frac{\partial^2}{\partial x_i \partial x_j} \psi_{\boldsymbol{k}} d\boldsymbol{x} \tag{29}$$

$$\approx \frac{\hbar^2}{m} \frac{\partial u_j}{\partial x_i} \sum_{\boldsymbol{k},\boldsymbol{k}'} C_{\boldsymbol{k}} e^{i\boldsymbol{k}'\cdot\boldsymbol{x}} \int \psi^*_{\boldsymbol{k}'} \frac{\partial^2 \psi_{\boldsymbol{k}}}{\partial x_i \partial x_j} d\boldsymbol{x} \tag{30}$$

$$\approx \frac{\hbar^2}{m} \frac{\partial u_j}{\partial x_i} \sum_{\boldsymbol{k},\boldsymbol{k}'} C_{\boldsymbol{k}} e^{i\boldsymbol{k}'\cdot\boldsymbol{x}} \int \psi^*_{\boldsymbol{o}} e^{-i\boldsymbol{k}'\cdot\boldsymbol{x}} \frac{\partial^2 (\psi_{\boldsymbol{o}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}})}{\partial x_i \partial x_j} d\boldsymbol{x} \tag{31}$$

$$= \frac{\hbar^2}{m} \frac{\partial u_j}{\partial x_i} \sum_{\boldsymbol{k},\boldsymbol{k}'} C_{\boldsymbol{k}} e^{i\boldsymbol{k}'\cdot\boldsymbol{x}} \int d\boldsymbol{x}\, e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{x}} \psi^*_{\boldsymbol{o}} \times \left( -k_i k_j \psi_{\boldsymbol{o}} + ik_i \frac{\partial \psi_{\boldsymbol{o}}}{\partial x_j} + ik_j \frac{\partial \psi_{\boldsymbol{o}}}{\partial x_i} + \frac{\partial^2 \psi_{\boldsymbol{o}}}{\partial x_i \partial x_j} \right) \tag{32}$$

$$= \frac{\hbar^2}{m} \frac{\partial u_j}{\partial x_i} \sum_{\boldsymbol{k},\boldsymbol{k}'} C_{\boldsymbol{k}} e^{i\boldsymbol{k}'\cdot\boldsymbol{x}} \delta_{\boldsymbol{k},\boldsymbol{k}'} ( -k_i k_j + ik_i \langle \partial_j \rangle + ik_j \langle \partial_i \rangle + \langle \partial_{ij} \rangle ) \tag{33}$$

$$= \frac{\hbar^2}{m} \frac{\partial u_j}{\partial x_i} \left( \frac{\partial^2}{\partial x_i \partial x_j} + \langle \partial_j \rangle \frac{\partial}{\partial x_i} + \langle \partial_i \rangle \frac{\partial}{\partial x_j} + \langle \partial_{ij} \rangle \right) F. \tag{34}$$

When $E(\boldsymbol{k}) = E_0 + \hbar^2 k_i k_j / 2m^*_{ij}$, the envelope function $F$ in a zero magnetic field is described by the next equation,

$$\left\{ -\frac{\hbar^2}{2m^*_{ij}} \frac{\partial^2}{\partial x_i \partial x_j} + \frac{\hbar^2}{2m} \left[ 2 \frac{\partial u_j}{\partial x_i} \left( \frac{\partial^2}{\partial x_i \partial x_j} + \langle \partial_j \rangle \frac{\partial}{\partial x_i} + \langle \partial_i \rangle \frac{\partial}{\partial x_j} + \langle \partial_{ij} \rangle \right) + \frac{\partial^2 u_j}{\partial x_i \partial x_i} \left( \frac{\partial}{\partial x_j} + \langle \partial_j \rangle \right) + \frac{\partial^2 u_j}{\partial x_i \partial x_j} \left( \frac{\partial}{\partial x_i} + \langle \partial_i \rangle \right) + \frac{1}{2} \frac{\partial^3 u_j}{\partial x_i \partial x_i \partial x_j} \right] + u_j \frac{\partial V_{\mathrm{ex}}}{\partial x_j} \right\} F = \mathcal{E}_{\mathrm{eff}} F. \tag{35}$$

Then the energies $E_\varepsilon \approx \mathcal{E}_{\mathrm{eff}} + E_0$, and the wave functions $\psi_\varepsilon \approx F\psi_{\boldsymbol{o}}$.

In order to confirm the effectiveness of the Hamiltonians, the numerical calculations are carried out using a one-dimensional strained Kronig-Penney model in a zero magnetic field. The strained potential is

$$V_\varepsilon(x) = \frac{3\pi\hbar^2}{2ma} \sum_{n=-\infty}^{\infty} \delta\{x - [na + u(na)]\}, \tag{36}$$

$$u(x) = 0.1 \times a \sin(2\pi x/10a), \tag{37}$$

where $\delta(x)$ is a delta function. Strain $u(x)$ is given as a sine wave, whose wavelength is ten times the unstrained lattice constant $a$, and whose amplitude is 10% of $a$. The exact solutions of this model are calculated by the conventional transfer-matrix method in Eqs. (10), (36), and (37). The energies $E_\varepsilon$ are indicated by black solid lines in Fig. 1, and the wave functions $|\psi_\varepsilon|^2$ are indicated in Fig. 2. The solutions of the Hamiltonian [Eqs. (12), (19), (37), and (38)] are calculated by diagonalizing the Hamiltonian matrix, and the energies $\mathcal{E}$ and the wave functions $|\mathcal{T}\phi|^2$ are indicated by red solid lines,

$$V_{\mathrm{st}}(x) = \frac{3\pi\hbar^2}{2ma} \sum_{n=-\infty}^{\infty} \delta(x - na), \quad V_{\mathrm{ex}}(x) = 0. \tag{38}$$

The solutions of the Hamiltonian in the improved effective-mass approximation [Eqs. (35) and (37)] are also calculated by diagonalizing the Hamiltonian matrix. The energies $\mathcal{E}_{\mathrm{eff}} + E_0$ and the wave functions $|F\psi_{\boldsymbol{o}}|^2$ are indicated by blue solid lines, and the envelope functions $|F|^2$ are indicated by blue broken lines. The Hamiltonians are accurate enough from the data in these figures, therefore I conclude that the proposed Hamiltonians are very valid.

Last, I would suggest that when the displacement is a time-dependent function $\boldsymbol{u}(\boldsymbol{x},t)$, it means the lattice vibration, that is, the phonons. Therefore the Hamiltonians can express the effects of phonons, also.

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