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DIFFERENT APPROACHES FOR MULTIBAND TRANSPORT IN SEMICONDUCTORS

РІЗНІ ПІДХОДИ ДО БАГАТОЗОННОГО ПЕРЕНОСУ В НАПІВПРОВІДНИКАХ

We compare the well-known Kane model with a new multiband envelope function model, which presents many advantages with respect to the first one.

Добре відому модель Кане порівняно з новою моделлю багатокомпонентної обвідної функції і продемонстровано багато переваг останньої.

1. Introduction. Multiband [1, 2] models are of paramount importance in nanometric semiconductor devices. In particular, we refer here to modeling interband tunneling, which is the main mechanism of working for some heterostructure devices (superlattices) like RITDs (Resonant Interband Tunneling Devices). In these superlattices the contact of heterogeneous semiconductor materials enables to obtain potential barriers that interface the conduction and the valence bands [3 – 6].

A quantum mechanics based model, able to treat a multiband dynamics [7 – 10] is the Kane model. Here we deal with the two-band case, to which some literature has been devoted (Wigner formulation, hydrodynamic formulation, ... [11 – 13]. The physical assumptions foresee a simplified environment, where magnetic and spin effects are disregarded. Dissipative phenomena like electron-phonon collisions are not taken into account. The dynamics of charge carriers is considered as confined in the two highest energy bands of the semiconductor, i.e., the conduction and the (nondegenerate) valence bands, around the point $\mathbf{k} = \mathbf{0}$, where $\mathbf{k}$ is the "crystal" wave vector. The point $\mathbf{k} = \mathbf{0}$ is assumed to be a minimum for the conduction band and a maximum for the valence band, in the parabolic approximation.

The Hamiltonian introduced in the Schrödinger equation is

$$H = H_0 + V, \qquad H_0 = -\frac{\hbar^2}{2m_0}\Delta + V_{\rm per}\,, \tag{1}$$

where $V_{\rm per}$ is the periodic potential of the crystal and V an "external" potential, which takes in account different effects, like the device energy-band offset for the heterojunctions, the bias voltage applied across the device, the contribution from the doping impurities and from the self-consistent field produced by the mobile electronic charge.

In this paper we compare the well-known Kane model to a new multiband envelope function model, which presents many advantages with respect to the first one. In Section 2 we recall the procedure of derivation of the Kane model from the Schrödinger equation and in Section 3 we describe the $\mathbf{k} \cdot \mathbf{P}$ method, which is the classical way of studying multiband systems governed by an Hamiltonian perturbed by an external potential [2, 14]. In Section 4 we propose a different procedure of approximation for the Schrödinger equation. Using again an expansion founded on the classical Bloch basis, the new strategy is separating the intraband dynamics terms from the interband coupling ones. The model obtained in such a way eventually contains interband terms and uses envelope functions which have, beyond other advantages, a direct physical interpretation. We observe that

the present paper is only a preliminary study for modeling interband tunneling effects. The reader interested in more details is referred to the forthcoming paper [15].

Finally, we claim that this paper, devoted to the modeling topics, is the first part of a wider project which foresees both analytical and numerical study of Schrödinger-like models, kinetic-like models (Wigner transform) and quantum hydrodynamic models for multiband systems.

2. Kane model. The equations system proposed (in a 3D infinite spatial domain) is the following:

$$\begin{aligned} i\hbar\frac{\partial\psi_c}{\partial t} &= -\frac{\hbar^2}{2m_0}\Delta\psi_c + (E_c+V)\psi_c - \frac{\hbar}{m_0}\,\mathbf{P}\cdot\boldsymbol{\nabla}\psi_v, \\ i\hbar\frac{\partial\psi_v}{\partial t} &= -\frac{\hbar^2}{2m_0}\Delta\psi_v + (E_v+V)\psi_v + \frac{\hbar}{m_0}\,\mathbf{P}\cdot\boldsymbol{\nabla}\psi_c, \end{aligned} \tag{2}$$

where ψ_c (ψ_v) is a conduction (valence) envelope function, m_0 is the bare mass of the carriers, $E_c(E_v)$ is the minimum (maximum) of the conduction (valence) band energy and $\mathbf{P}$ is the coupling term between the two bands, which represents the momentum operator matrix element between the corresponding (conduction and valence) Wannier functions. In general $\mathbf{P}$ depends on the effective mass tensor and on the energy gap between the bands. Introducing

$$\boldsymbol{\Psi} \equiv \begin{pmatrix} \psi_c \\ \psi_v \end{pmatrix}, \qquad \mathcal{H}_{\mathbf{K}} \equiv \begin{pmatrix} -\dfrac{\hbar^2}{2m_0}\Delta + E_c + V & -\dfrac{\hbar}{m_0}\,\mathbf{P}\cdot\boldsymbol{\nabla} \\ \dfrac{\hbar}{m_0}\,\mathbf{P}\cdot\boldsymbol{\nabla} & -\dfrac{\hbar^2}{2m_0}\Delta + E_v + V \end{pmatrix}, \tag{3}$$

we can rewrite (2) in a vectorial notation

$$i\hbar\frac{\partial\boldsymbol{\Psi}}{\partial t} = \mathcal{H}_K\boldsymbol{\Psi}\ . \tag{4}$$

$\mathcal{H}_K$ is known as the Kane – Hamiltonian and the extension of (4) to the n-band case is straightforward.

We recall here briefly the procedure of derivation of (2) from the Schrödinger equation for an electron subjected to a periodic potential plus an external potential V, which writes as

$$i\hbar\frac{\partial\Psi}{\partial t} = (H_0+V)\Psi\ , \tag{5}$$

where Ψ represents the wave function of the electron.

We perform the expansion of a generic solution Ψ on a Bloch basis, considering all the bands

$$\Psi(\mathbf{x}) = \sum_n \int\limits_B d\mathbf{k}\,\varphi_n(\mathbf{k})b_n(\mathbf{k},\mathbf{x}), \quad n=1,2,\dots\ , \tag{6}$$

where B is the first Brillouin zone and the eigenfunctions of H_0, i.e., the Bloch eigenfunctions, can be written as

$$b_n(\mathbf{k},\mathbf{x}) = \mathrm{e}^{i\,\mathbf{k}\cdot\mathbf{x}}u_n(\mathbf{k},\mathbf{x}) \equiv \langle\mathbf{x}|n,\mathbf{k}\rangle\ . \tag{7}$$

We consider as a new basis the periodic part of Bloch functions, i.e., $u_n(\mathbf{k},\mathbf{x})$, at $\mathbf{k}=\mathbf{0}$ and perform the expansion

$$u_n(\mathbf{k},\mathbf{x}) = \sum_{n'} \mathcal{C}_{n,n'}(\mathbf{k}) u^0_{n'}(\mathbf{x}), \tag{8}$$

where $u^0_{n'}(\mathbf{x}) = u_{n'}(\mathbf{0},\mathbf{x})$.

Using as a basis $u^0_{n'}(\mathbf{x})$ in (6), $\Psi(\mathbf{x})$ reads as

$$\Psi(\mathbf{x}) = \sum_n \psi_n(\mathbf{x}) u^0_n(\mathbf{x}) \ , \tag{9}$$

where the functions

$$\psi_n(\mathbf{x}) = \sum_{n'} \int\limits_B d\mathbf{k}\, \varphi_{n'}(\mathbf{k}) \mathcal{C}_{n,n'}(\mathbf{k}) \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}}, \quad n, n' = 1, 2, \ldots, \tag{10}$$

are "Kane" envelope functions, which do not depend on $\mathbf{k}$ anymore. In a two-band dynamics ($n, m = c, v$, where c stands for "conduction band" and v stands for "valence band") expansion (6) takes the form

$$\Psi(\mathbf{x}) = \psi_c(\mathbf{x}) u^0_c(\mathbf{x}) + \psi_v(\mathbf{x}) u^0_v(\mathbf{x}) \ , \tag{11}$$

which is the envelope function expansion of the wave function Ψ that leads to **Kane model** (2).

Summarizing the preceding considerations, we remark that the Kane model is derived introducing a new basis (constructed around $\mathbf{k} = \mathbf{0}$). The "Kane" basis functions are not eigenfunctions of the unperturbed Hamiltonian. The "Kane" basis corresponds to a rotation of the Bloch basis

$$u^0_n(\mathbf{x}) = \sum_{n'} \mathcal{C}^{-1}_{n,n'}(\mathbf{k}) u_{n'}(\mathbf{k},\mathbf{x}) \ . \tag{12}$$

We conclude the section highlighting some defect and shortcoming produced by the approximations performed on the way of Kane model's derivation. First, the potential V affects the band energy terms, but it does not appear in the coupling term $\mathbf{P}$; second, there is an interband coupling even in absence of an external potential; third, the interband term $\mathbf{P}$ increases when the energy gap between the two bands E_g increases (the opposite of physical evidence); fourth there is no direct physical interpretation of "conduction" and "valence" electron envelope functions. These considerations convince us, beyond the sure merits of Kane model, to investigate a different approximation approach to the Schrödinger equation, in order to attain a more physically consistent model.

3. Luttinger – Kohn model. We now briefly describe the $\mathbf{k}\cdot\mathbf{P}$ technique [2], which is successfully used to analyze the electronic properties of a wide type of semiconductor. The spirit of a $\mathbf{k}\cdot\mathbf{P}$ model is to use momentum $\mathbf{k}$ as a perturbation parameter of the Hamiltonian.

If we write the eigenvalue equation for the semiconductor without external field, we have

$$H_0 b_n(\mathbf{k},\mathbf{x}) = E_n(\mathbf{k}) b_n(\mathbf{k},\mathbf{x}),$$

where $b_n(\mathbf{k},\mathbf{x})$ are the Bloch functions in (7). It easy to show that the eigenvalue equation solved by the periodic part of Bloch function $u_n(\mathbf{k},\mathbf{x})$ is now:

$$(H_0 + H')u_n(\mathbf{k}, \mathbf{x}) =$$
$$= \left[-\frac{\hbar^2}{2m_0}\Delta - i\frac{\hbar^2}{m_0}(\mathbf{k}\cdot\boldsymbol{\nabla}) + \frac{\hbar^2 k^2}{2m_0} + V_{\mathrm{per}}(\mathbf{x}) \right] u_n(\mathbf{k}, \mathbf{x}) =$$
$$= E_n(\mathbf{k})u_n(\mathbf{k}, \mathbf{x}) \ ,$$

where $k = |\mathbf{k}|$. Here $H_0 + H'$ is the so-called $\mathbf{k}\cdot\mathbf{P}$ Hamiltonian, where H_0 is the single electron Hamiltonian (1) and

$$H' = -i\frac{\hbar^2}{m_0}(\mathbf{k}\cdot\ \boldsymbol{\nabla}\ ) + \frac{\hbar^2 k^2}{2m_0}$$

is an additional term which is treated as a perturbation, since it vanishes when $\mathbf{k} \to 0$. Thus, for states localized near the center of the (first) Brillouin zone, H' is small and the original problem is faced first solving the unperturbed problem

$$H_0 u_n(\mathbf{0}, \mathbf{x}) = E_n(\mathbf{0})u_n(\mathbf{0}, \mathbf{x})$$

and then using the perturbation H' to get some correction on $E_n(\mathbf{0})$ and $u_n(\mathbf{0}, \mathbf{x})$ when $\mathbf{k} \neq \mathbf{0}$. The non degenerate perturbation theory provides that, at the first order of the perturbation H', the eigenfunctions for the perturbed problem are

$$u_n^1(\mathbf{0}, \mathbf{x}) = u_n^0(\mathbf{x}) + \mathbf{k}\cdot\boldsymbol{\nabla}_k u_n(\mathbf{k}, \mathbf{x})\Big|_{\mathbf{k}=0} =$$

$$= u_n^0(\mathbf{x}) - \frac{\hbar}{m_0}\sum_{n'\neq n}\frac{\mathbf{k}\cdot\mathbf{P}_{n,n'}}{\triangle E_{n,n'}}\ u_{n'}(\mathbf{0}, \mathbf{x}),$$

with

$$\triangle E_{n,n'} = E_n(\mathbf{0}) - E_{n'}(\mathbf{0})$$

and

$$\mathbf{P}_{n,n'} \equiv \frac{(2\pi)^3}{\Omega}\int\limits_{u-\mathrm{cell}} d\mathbf{x}\, u_n^*(\mathbf{0}, \mathbf{x})\,\boldsymbol{\nabla}\, u_{n'}(\mathbf{0}, \mathbf{x}), \tag{13}$$

where Ω is the volume of the unitary cell $(u - \mathrm{cell})$. In this way, using perturbation theory, we are driven to work with a (non orthonormal) basis, that arises from the following quasiunitary rotation operator Θ, applied to the unperturbed $(u_n^0(\mathbf{x}))$ basis

$$u_n^1(k, \mathbf{x}) = \sum_{n'}\Theta_{n,n'}(\mathbf{k})u_{n'}^0(\mathbf{x}),$$

with

$$\Theta_{n,n'}(\mathbf{k}) = \left(\delta_{n,n'} - \frac{\hbar}{m_0}\frac{\mathbf{k}\cdot\mathbf{P}_{n,n'}}{\triangle E_{n,n'}}\right).$$

Luttinger and Kohn [14] proposed to apply the previous procedure to the Kane Hamiltonian $\mathcal{H}_K$ (3) in the n-band case (where the basis elements are the unperturbed elements $u_n^0(\mathbf{x})$), diagonalizing it to the first order in k. Using Fourier transform, we can recast the system (4) in the following way:

$$\left(E_n + \frac{\hbar^2 k^2}{2m_0}\right)\widetilde{\psi}_n(\mathbf{k}) + \frac{\hbar}{m_0}\sum_{n'}\mathbf{k}\cdot\mathbf{P}_{n,n'}\widetilde{\psi}_{n'}(\mathbf{k}) + \int_B d\mathbf{k}'\,\widetilde{V}(\mathbf{k}-\mathbf{k}')\widetilde{\psi}(\mathbf{k}') = 0,$$

where $\widetilde{\psi}_n(\mathbf{k})$, $\widetilde{V}(\mathbf{k})$ are the Fourier transform of $\psi_n(\mathbf{x})$, $V(\mathbf{x})$ respectively. If we operate the following change of variable

$$\widetilde{\chi}_n = \sum_{n'} \Theta^{-1}_{n,n'}\, \widetilde{\psi}_{n'}$$

and we go back to the coordinate space, we recover the Luttinger – Kohn system. The authors proposed to neglect all off-diagonal term, and thus they achieved the following uncoupled equations set, for a 3D spatial domain (conduction-valence, i.e., the two-band case):

$$\begin{aligned} i\hbar\frac{\partial \chi_c}{\partial t} &= E_c\chi_c - \frac{\hbar^2}{2m_c^*}\Delta\chi_c + V\chi_c, \\ i\hbar\frac{\partial \chi_v}{\partial t} &= E_v\chi_v + \frac{\hbar^2}{2|m_v^*|}\Delta\chi_v + V\chi_v\ , \end{aligned} \tag{14}$$

where m_c^* and m_v^* are, respectively, the isotropic effective mass in the conduction and valence bands, given by the following expression:

$$\frac{m_0}{m_n^*} = 1 - \frac{2\hbar^2}{3m_0}\sum_{n'\neq n}\frac{\mathbf{P}_{n,n'}\cdot\mathbf{P}_{n',n}}{\triangle E_{n,n'}}\ ,$$

where m_0 is the bare mass of the electron, n denotes the band index (in the two-band case $n = c, v$) and n' runs on all the other bands. As it is manifest, disregarding the off-diagonal terms implies the achievement of two uncoupled equations for the envelope functions in the two bands. This means that the model, at this stage of approximation, is not able to describe an interband tunneling dynamics.

4. A different approach. In this section we propose a different procedure of approximation for the Schrödinger equation (5), under the same physical assumptions used in the Kane model [15].

If we expand equation (5) using the Bloch basis $b_n(\mathbf{k}, \mathbf{x})$ like in (6), we obtain n-equations for the expansion coefficients

$$\begin{aligned} i\hbar\frac{\partial \varphi_n}{\partial t}(\mathbf{k}) = E_n(\mathbf{k})\varphi_n(\mathbf{k}) + \\ + \sum_{n'}\int\limits_B d\mathbf{k}'\,\langle n,\mathbf{k}|V|n',\mathbf{k}'\rangle\varphi_n(\mathbf{k}'), \quad n = 1, 2, \dots\ . \end{aligned} \tag{15}$$

Equations (15) are exact but of no practical utility. In order to provide suitable approximations and attain a model which still maintain interband dynamics terms, but which is less tough to handle, we separate the **intraband dynamics** from the **interband coupling**. After some algebra we get

$$\begin{aligned} i\hbar\frac{\partial \varphi_n}{\partial t}(\mathbf{k}) = E_n(\mathbf{k})\varphi_n(\mathbf{k}) + \int\limits_B d\mathbf{k}'\,\widetilde{V}(\mathbf{k}-\mathbf{k}')\varphi_n(\mathbf{k}') - \\ -i\frac{\hbar^2}{m_0}\sum_{n'\neq n}\int\limits_B d\mathbf{k}'\,\widetilde{V}(\mathbf{k}-\mathbf{k}')\varphi_{n'}(\mathbf{k}')\frac{(2\pi)^3}{\Omega}\times \\ \times\int\limits_{u-\mathrm{cell}} d\mathbf{x}\,u_n^*(\mathbf{k},\mathbf{x})\frac{\mathbf{k}-\mathbf{k}'}{\triangle E_{n,n'}}\cdot\boldsymbol{\nabla}u_{n'}(\mathbf{k}',\mathbf{x}), \end{aligned} \tag{16}$$

where $\widetilde{V}$ denotes the Fourier transform of the potential V and

$$\triangle E_{n,n'}(\mathbf{k},\mathbf{k}') \equiv E_{n'}(\mathbf{k}') - E_n(\mathbf{k}) + \frac{\hbar^2}{2m_0}\left(k'^2 - k^2\right). \tag{17}$$

This new set of n-equations is so far very general and only relies on the assumption that the potential V has no appreciable variation on the scale of a single lattice cell. The approximation procedure that we have chosen is based on three steps.

First, simplify the interband term to the lowest order in k:

$$-i\sum_{n'\neq n}\frac{\hbar^2\mathbf{P}_{n,n'}}{m_0\triangle E_{n,n'}}\int\limits_B d\mathbf{k}'\left(\mathbf{k}-\mathbf{k}'\right)\widetilde{V}(\mathbf{k}-\mathbf{k}')\varphi_{n'}(\mathbf{k}'). \tag{18}$$

Second, introduce the effective mass approximation

$$E_n(\mathbf{k}) = E_n + \frac{\hbar^2 k^2}{2m_n^*} + \cdots\ , \tag{19}$$

where m_n^* is the isotropic effective mass in the n-band.

Third and final, obtain the equations for the envelope functions in the coordinates space by inverse Fourier transform.

This result can be attained by projection of the wave function on the Wannier basis ϕ_n^W which depends on $(\mathbf{x}-\mathbf{R}_i)$, where $\mathbf{R}_i$ are the atomic sites positions, i.e.,

$$\Psi(\mathbf{x}) = \sum_n\sum_{\mathbf{R}_i}\chi_n(\mathbf{R}_i)\phi_n^W(\mathbf{x}-\mathbf{R}_i)\ , \tag{20}$$

where the Wannier basis functions can be expressed in terms of Bloch functions as

$$\phi_n^W(\mathbf{x}-\mathbf{R}_i) = \sqrt{\frac{\Omega}{(2\pi)^3}}\int\limits_B b_n(\mathbf{k},\mathbf{x}-\mathbf{R}_i)d\mathbf{k}\ . \tag{21}$$

The use of the Wannier basis has some advantages. As a matter of fact the amplitudes $\chi_n(\mathbf{R}_i)$, that play the role of envelope functions on the new basis, can be obtained from the Bloch coefficients (see (15)) by a simple Fourier transform

$$\chi_n(\mathbf{R}_i) = \sqrt{\frac{\Omega}{(2\pi)^3}}\int\limits_B \varphi_n(\mathbf{k})\mathrm{e}^{i\mathbf{k}\cdot\mathbf{R}_i}d\mathbf{k}. \tag{22}$$

Moreover they can be interpreted as the actual wave function of an electron in the n-band. In fact, "macroscopic" properties of the system, like charge density and current, can be expressed in term of $\chi_n(\mathbf{R}_i)$, averaging on a scale of the order of the lattice cell.

Performing the limit to the continuum by extending the dependence of the $\chi_n(\mathbf{R}_i)$ to the whole space $(\mathbf{R}_i \longrightarrow \mathbf{x})$ and by using standard properties of the Fourier transform, equations for the coefficients $\chi_n(\mathbf{x})$ are achieved.

In case of only two bands ("conduction" and "valence") the equations for the envelope functions take the form

$$\begin{aligned} i\hbar\frac{\partial\chi_c}{\partial t} &= -\frac{\hbar^2}{2m_c^*}\Delta\chi_c + V\chi_c + E_c\chi_c - \frac{\hbar^2\mathbf{P}\cdot\boldsymbol{\nabla}V}{m_0E_g}\chi_v,\\ i\hbar\frac{\partial\chi_v}{\partial t} &= \frac{\hbar^2}{2|m_v^*|}\Delta\chi_v + V\chi_v + E_v\chi_v - \frac{\hbar^2\mathbf{P}\cdot\boldsymbol{\nabla}V}{m_0E_g}\chi_c. \end{aligned} \tag{23}$$

These equations describe the intraband dynamics in the effective mass approximation in the same fashion as the Luttinger – Kohn model, but also contain an interband coupling, proportional to the momentum matrix element $\mathbf{P}$, that is responsible for tunneling between different bands induced by the applied electric field proportional to the x-derivative of V. As discussed above, the envelope functions χ_c and χ_v are the projections of the full wavefunction ψ on the Wannier basis, and therefore represent the (cell-averaged) probability amplitude for finding an electron on the conduction or valence bands (of the unperturbed problem) respectively. This "natural" choice of the basis allows in principle for a clear and systematic expansion at higher orders in k, and has important advantages with respect to the Kane approach. Indeed, as one would naively expect, in this case the interband coupling term reduces as the energy gap E_g increases, and vanishes in the absence of the external field V.

This opens the interesting perspective of comparing the predictions of the Kane model and the model in equation (23) for semiconductor devices where interband tunneling effects plays a major role, like in RITDs.

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