"Recent Trends in Kinetic Theory and its Applications"
KYIV, Ukraine, May 11-15, 2004

Different approaches for multi-band transport in semiconductors

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Introduction

Quantum aspects become predominant in some of the most recent 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 Tunnel Devices). In these superlattices the contact of heterogeneous semiconductor materials enables to obtain potential barriers that interface the conduction and the valence band.

A quantum mechanics based model (**Kane** model) is rather widely used and studied in literature (Wigner formulation, hydrodynamic formulation ...).

The physical environment

Electromagnetic and spin effects are disregarded, just like the field generated by the charge carriers themselves. 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 (non–degenerate) valence band, 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. The parabolic approximation is considered as valid.
The Hamiltonian introduced in the Schrödinger equation is

$$H = H_0 + V \,, \quad H_0 = -\frac{\hbar^2}{2m}\Delta + V_{per} \,,$$

where V_{per} is the periodic potential of the crystal and V an external potential.

Kane Model

The equations system proposed is the following:

$$\begin{cases} i\hbar\dfrac{\partial\psi_c}{\partial t} &= -\dfrac{\hbar^2}{2m}\Delta\psi_c + V_c\psi_c + \dfrac{\hbar}{m}P\nabla\psi_v \\ i\hbar\dfrac{\partial\psi_v}{\partial t} &= -\dfrac{\hbar^2}{2m}\Delta\psi_v + V_v\psi_v - \dfrac{\hbar}{m}P\nabla\psi_c\ , \end{cases} \tag{1}$$

- m is the bare mass of the carriers,
- V_c (V_v) is the minimum (maximum) of the conduction (valence) band energy
- P is the coupling coefficient between the two bands. In a one-dimension model $P = \frac{m}{\hbar}\sqrt{\frac{m-m^*}{2mm^*}E_g}$, where m^* is the effective mass and $E_g = V_c - V_v$ is the energy gap between the two bands.

Preliminary remark on Kane model

- The external potential V affects the band energy terms V_c (V_v), but it does not appear in the coupling coefficient P;

- There is an interband coupling even in absence of an external potential;

- The interband coefficient P increases when the energy gap between the two bands E_g increases (the opposite of physical evidence.

Derivation of Kane model

Schrödinger equation for an electron in a periodic potential plus an external potential V

$$i\hbar\partial_t \Psi = (H_0 + V)\Psi \tag{2}$$

Expansion of a generic solution on a Bloch basis

$$\Psi(\mathbf{x}) = \sum_n \int_B \varphi_n(\mathbf{k}) b_n(\mathbf{k}, \mathbf{x}) d\mathbf{k} \tag{3}$$

- B is the first Brillouin zone.

Bloch eigenfunctions

$$b_n(\mathbf{k}, \mathbf{x}) = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}} u_n(\mathbf{k}, \mathbf{x}) \equiv |n, \mathbf{k}\rangle \tag{4}$$

Consider as a new basis the periodic part of Bloch functions, $u_n(\mathbf{k},\mathbf{x})$ at $\mathbf{k}=\mathbf{0}$.

Perform the expansion

$$u_n(\mathbf{k},\mathbf{x}) = \sum_{n'=1}^{\infty} \mathcal{C}_{nn'}(\mathbf{k}) u^o_{n'}(\mathbf{x}) \tag{5}$$

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

Introduce in (3):

$$\Psi(\mathbf{x}) = \sum_{n=1}^{\infty} \psi_n(\mathbf{x}) u^o_n(\mathbf{x}) \ , \tag{6}$$

where the functions

$$\psi_n(\mathbf{x}) = \int_B \sum_{n'=1}^{\infty} \varphi_{n'}(\mathbf{k}) \mathcal{C}_{nn'}(\mathbf{k}) \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}} \, d\mathbf{k} \ , \ \ n = 1,2,\ldots, \tag{7}$$

are "Kane " envelope functions and do not depend on $\mathbf{k}$.

In a two-band dynamics, then $n, m = c, v$ where c stands for "conduction band" and v stands for "valence band".
Expansion (6) becomes

$$\Psi(\mathbf{x}) = \psi_c(\mathbf{x}) u_c^o(\mathbf{x}) + \psi_v(\mathbf{x}) u_v^o(\mathbf{x}) \tag{8}$$

which is the envelope function expansion of the wave function Ψ that leads to **Kane model** (1).

A different approach

Recall the expansion (3) of a generic solution of the Schrödinger equation (2) on a Bloch basis

$$\Psi(\mathbf{x}) = \sum_n \int_B \varphi_n(\mathbf{k}) b_n(\mathbf{k}, \mathbf{x}) d\mathbf{k}$$

where the Bloch eigenfunctions are

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

Equation for the expansion coefficients

$$i\hbar\partial_t \varphi_n(\mathbf{k}) = E_n(\mathbf{k})\varphi_n(\mathbf{k}) + \sum_{n'} \int_B \langle n, \mathbf{k}|V|n', \mathbf{k}'\rangle \varphi_n(\mathbf{k}') d\mathbf{k}' d\mathbf{k}' \qquad (9)$$

Let us separate the **intraband dynamics** from the **interband coupling**; after some algebra we get

$$i\hbar\partial_t\varphi_n(\mathbf{k}) = E_n(\mathbf{k})\varphi_n(\mathbf{k}) + \int_B \tilde{V}(\mathbf{k}-\mathbf{k}')\varphi_n(\mathbf{k}')d\mathbf{k}' \tag{10}$$

$$-i\frac{\hbar^2}{m}\sum_{n'\neq n}\int_B \frac{\mathbf{k}-\mathbf{k}'}{\Delta E_{n,n'}}\tilde{V}(\mathbf{k}-\mathbf{k}')\varphi_{n'}(\mathbf{k}')d\mathbf{k}'\frac{(2\pi)^3}{\Omega}\int_{u-cell} u_n^*(\mathbf{k},\mathbf{x})\nabla u_{n'}(\mathbf{k}',\mathbf{x})d\mathbf{x}$$

where $\tilde{V}$ denotes the Fourier transform of the external potential and where we have defined

$$\Delta E_{n,n'} = \Delta E_{n,n'}(\mathbf{k},\mathbf{k}') \equiv E_{n'}(\mathbf{k}') - E_n(\mathbf{k}) + \frac{\hbar^2}{2m}\left(k'^2 - k^2\right) \tag{11}$$

where $k = |\mathbf{k}|$

This equation is so far very general and only relies on the assumption that the external potential V has no appreciable variation on the scale of a single lattice cell.

Our aim: simplify the above equation and write it in coordinate space.

1. Simplify the interband term:

$$-i \sum_{n' \neq n} \frac{\hbar^2 P_{n,n'}}{m \Delta E_{n,n'}(0)} \int_B \left(\mathbf{k} - \mathbf{k'} \right) \tilde{V}(\mathbf{k} - \mathbf{k'}) \varphi_{n'}(\mathbf{k'}) d\mathbf{k'} \tag{12}$$

with

$$P_{n,n'} \equiv \frac{(2\pi)^3}{\Omega} \int_{u-cell} u_n^*(\mathbf{0}, \mathbf{x}) \nabla u_{n'}(\mathbf{0}, \mathbf{x}) x \mathbf{x} \tag{13}$$

2. Effective mass approximation:

$$E_n(\mathbf{k}) = E_n + \frac{\hbar^2 k^2}{2 m_n^*} + \cdots \tag{14}$$

3. keep the $u_n(\mathbf{k},\mathbf{x})$ to first order in $\mathbf{k}$ in the interband term, i.e. use as a basis

$$u(\mathbf{0},\mathbf{x}) + \mathbf{k}\frac{\partial u(\mathbf{k},\mathbf{x})}{\partial \mathbf{k}}\bigg|_{\mathbf{k}=\mathbf{0}} .$$

4. obtain the equations for the envelope functions by inverse Fourier transform.

Remark

More rigorously, by projection on the Wannier basis

$$\Psi(\mathbf{x}) = \sum_n \sum_{\mathbf{R}_i} \chi_n(\mathbf{R}_i)\phi_n^W(\mathbf{x}-\mathbf{R}_i) \tag{15}$$

which can be expressed in terms of Bloch funtions as

$$\phi_n^W(\mathbf{x}-\mathbf{R}_i) = \sqrt{\frac{\Omega}{(2\pi)^3}}\int_k b_n(\mathbf{k},\mathbf{x}-\mathbf{R}_i). \tag{16}$$

The use of the Wannier basis has two advantages:

(i) the amplitudes $\chi_n(\mathbf{R}_i)$, that play the role af envelope functions on the new basis can be obtained from the Bloch coefficients in Eq. (3) by a simple Fourier transform

$$\chi_n(\mathbf{R}_i) = \sqrt{\frac{\Omega}{(2\pi)^3}} \int_B \varphi_n(\mathbf{k}) \mathrm{e}^{i\mathbf{k}\cdot\mathbf{R}_i} d\mathbf{k}; \tag{17}$$

(ii) they can be interpreted as the actual wave function of an electron in the nth band if one is interested in "macroscopic" properties of the system on a scale much larger that the lattice spacing (that is equivalent to average 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 ($\mathbf{R}_i \longrightarrow \mathbf{x}$), 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 equation for the envelope functions take the form

$$i\hbar\partial_t\chi_c(\mathbf{x}) = E_c\chi_c(\mathbf{x}) - \frac{\hbar^2}{2m_c^*}\Delta\chi_c(\mathbf{x}) + V(\mathbf{x})\chi_c(\mathbf{x}) - \nabla V(\mathbf{x})\frac{\hbar^2 P}{mE_g}\chi_v(\mathbf{x})$$

$$i\hbar\partial_t\chi_v(\mathbf{x}) = E_v\chi_v(\mathbf{x}) - \frac{\hbar^2}{2m_v^*}\Delta\chi_v(\mathbf{x}) + V(\mathbf{x})\chi_v(\mathbf{x}) - \nabla V(\mathbf{x})\frac{\hbar^2 P}{mE_g}\chi_c(\mathbf{x})$$

Final remarks on Kane model

- Kane model is constructed introducing a new basis (constructed around $\mathbf{k} = \mathbf{0}$)

$$\psi_n^{Kane}(\mathbf{k}, \mathbf{x}) = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}} u_n(\mathbf{0}, \mathbf{x}) \tag{18}$$

- the "Kane" basis functions are not eigenfunctions of the unperturbed Hamiltonian; the the "Kane" basis correspond to a rotation of the Bloch basis

$$u_n(\mathbf{0}, \mathbf{x}) = \sum_{n,n'} a_{n,n'}(\mathbf{k}) u_m(\mathbf{k}, \mathbf{x}) \tag{19}$$

- interband coupling even in the absence of an external potential: there is no direct physical interpretation of "conduction" and "valence" electrons;

- this means that in principle the "Bloch method" and the "Kane model" are different in the case of two bands: in the Bloch case the intraband effects can be fully included by releasing the effective mass approximation (and approximating only the coupling term due to the external potential), while in the case of the Kane model the intraband effects are anyhow truncated.