A "SPINORIAL" WIGNER FUNCTION DESCRIBING THE TWO-BAND K·P DYNAMICS OF ELECTRONS IN CRYSTALS*

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We study the two-band k·p model of electron transport in periodic potentials by means of a spinorial Wigner function, resulting from the decomposition of the Wigner matrix into Pauli-matrices components. The physical informations contained into the four Wigner functions obtained in this way, as well as their dynamics and local balance laws, are discussed.

1. Introduction

The recent, extraordinary achievements of nano-technologies made possible to conceive, and in many cases realize, electronic devices based on purely quantum principles. The usual semiclassical approach to charge transport in semiconductors is not sufficient any more to describe such a new generation of devices and, correspondingly, quantum transport theory is becoming quite a popular subject in the community of engineers, mathematicians and physicists interested in semiconductor devices.

The quantum dynamics of an electron in a semiconductor crystal (or, in general, of a particle in a periodic potential) is described by a Hamiltonian operator of the following form:

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

where m is the electron "bare" mass, $V_{\rm per}$ is the periodic potential generated by the ions of the crystal lattice and V is the non-periodic part of

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the potential (accounting e.g. for doping and/or external bias). Note that here we are neglecting lattice vibrations (phonons), electron-electron interactions and heterostructure effects, i.e. step-like potentials appearing at the interfaces between two layers of different semiconductor materials (we shall briefly comment on this in Remark 1.1).

Even in such a simplified framework, the Hamiltonian (1) is, in general, far too complicated for modeling purposes. Rather, it can be used to deduce simpler approximated models. The simplest of such models is given by the "effective-mass Hamiltonian", which has the following form:

$$H_{\rm em} = -\frac{\hbar^2}{2}\,\nabla^{\rm T}\mathbb{M}^{-1}\nabla + V. \tag{2}$$

Here, the effect of the periodic potential $V_{\rm per}$ is approximately taken into account by the effective-mass tensor $\mathbb{M}$, arising from a parabolic approximation of the energy band under consideration (conduction/valence) near an extremum point.[1] The physical meaning of such approximation is that a particle in a periodic potential behaves, in first approximation, as a free particle with a different (and, possibly, direction-dependent) mass. The simple form of $H_{\rm em}$ implies that, in the effective-mass approximation, the charge carrier "sees" only its typical energy band (conduction for electrons, valence for holes). For this reason such model is unable to describe effects, like the *interband tunneling*, that become very important when, due to the particular device architecture, two or more bands of the energy spectrum are actually available to the carrier.

A refined model, capable to describe the effect of two bands, is the so-called *two-band k·p Hamiltonian*[2] (sometimes referred to as the "Kane Hamiltonian"), which has the following form:

$$H_{\rm kp} = \begin{pmatrix} -\frac{\hbar^2}{2m}\Delta + E_g + V & -\frac{\hbar^2}{m}\,K\cdot\nabla \\ \\ \frac{\hbar^2}{m}\,K\cdot\nabla & -\frac{\hbar^2}{2m}\Delta + V \end{pmatrix}. \tag{3}$$

Note that, here, the effect of the periodic potential is taken into account by the parameters E_g, which is the so called *direct energy-gap*, and $K = (K_1, K_2, K_3)$, which is the matrix element of the gradient operator between the Bloch functions of the two bands[1,2]

$$K = \int\limits_{lattice\ cell} u_{\rm c}(x)\nabla u_{\rm v}(x)\,dx$$

(here and in the following, the subscripts c and v stand for *conduction* and *valence*).

Remark 1.1. We have already mentioned that here we are neglecting heterostructure potentials, assuming to be dealing with a "bulk crystal". This implies that the parameters E_g and K are constant. In the engineering literature it is customary to introduce heterostructure potentials by simply letting E_g depend on the space variable. Moreover, we are also neglecting electron-electron interactions: these can be approximately taken into account by letting the external potential V depend self-consistently by the electron density, through a Poisson equation.

In the following we shall study the quantum system described by Hamiltonian (3) in the framework of the Wigner formulation of quantum mechanics.[3,4,5,6] There are at least two good reasons for this choice. The first one is that the Wigner formalism is particularly suited to *quantum statistics* (and it is clear that one needs quantum statistics when dealing with a flow of many electrons through a device). The second reason is that the Wigner function 'tries very hard to be a joint density for momentum and position[5]'. Thus, Wigner functions allow a "quasi-kinetic" formulation of quantum mechanics and this makes the physical content of the Wigner picture be somehow more intuitive than that of the density-matrix picture.

The following analysis is inspired by the Wigner-function analysis of spin systems;[7] however, to the best of our knowledge, the application of these techniques to k·p Hamiltonians is new.

2. The spinorial Wigner function

The two-band k·p Hamiltonian (3) acts in the Hilbert space $\mathcal{H} := L^2(\mathbb{R}^3, \mathbb{C}^2)$, whose unitary elements $\psi = (\psi_1, \psi_2) \in \mathcal{H}$ represent the pure states of the system (wave functions). The mixed states of the system are represented by self-adjoint, positive and trace-class operators on $\mathcal{H}$, called *density operators*. Any density operator S admits a unique integral representation

$$(S\psi)_i = \sum_{j=1}^{2} \int_{\mathbb{R}^3} \rho_{ij}(x,y)\psi(y)\, dy,$$

where $\boldsymbol{\rho} = (\rho_{ij})$ is called the *density matrix* associated to the mixed state[4]. The *Wigner matrix* $\boldsymbol{w} = (w_{ij})$ associated to $\boldsymbol{\rho}$ is defined by[7,8,9]

$$w_{ij}(r,p) := \frac{1}{(2\pi\hbar)^3} \int_{\mathbb{R}^3} \rho_{ij}\Big(r + \frac{\xi}{2}, r - \frac{\xi}{2}\Big)\, \mathrm{e}^{-i\xi\cdot p/\hbar}\, d\xi, \tag{4}$$

for $i,j = 1,2$ and $(r,p) \in \mathbb{R}^3 \times \mathbb{R}^3$. The mapping $\boldsymbol{\rho} \mapsto \boldsymbol{w}$ is the *Wigner transformation*[3,4,5,6] and turns out to be a unitary transformation of $L^2(\mathbb{R}^3 \times \mathbb{R}^3, \mathbb{C}^{2,2})$ into itself. Moreover, the self-adjointness of the density operator S, which is reflected by the property $\rho_{ij}(x,y) = \overline{\rho_{ji}(y,x)}$ of the density matrix $\boldsymbol{\rho}$, implies that the Wigner matrix $\boldsymbol{w}$ is a 2×2 complex, hermitian matrix for any fixed (r,p):

$$\boldsymbol{w}(r,p) = \boldsymbol{w}^*(r,p), \quad (r,p) \in \mathbb{R}^3 \times \mathbb{R}^3. \tag{5}$$

Thus, recalling that the Pauli matrices

$$\boldsymbol{\sigma}_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \boldsymbol{\sigma}_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

are a orthonormal basis of the real vector space of 2×2 hermitian matrices with respect to the scalar product $(A,B) = \frac{1}{2}\,\mathrm{tr}\,(AB)$, we can uniquely decompose the Wigner matrix $\boldsymbol{w}$ with respect to such basis:

$$\boldsymbol{w}(r,p) = \sum_{k=0}^{3} w_k(r,p)\,\boldsymbol{\sigma}_k, \quad (r,p) \in \mathbb{R}^3 \times \mathbb{R}^3, \tag{6}$$

where the functions $w_k = w_k(r,p)$ are real-valued for $k = 0,1,2,3$. These will be the four Wigner functions associated to our physical system.

Proposition 2.1. *Let* $\langle w_k \rangle(r) := \int_{\mathbb{R}^3} w_k(r,p)\,dp$ *be the "local average" of* w_k. *Then*

$$\begin{aligned} \langle w_0 \rangle^2 &= \langle w_1 \rangle^2 + \langle w_2 \rangle^2 + \langle w_3 \rangle^2, \quad \textit{for a pure state,} \\ \langle w_0 \rangle^2 &\geq \langle w_1 \rangle^2 + \langle w_2 \rangle^2 + \langle w_3 \rangle^2, \quad \textit{for a mixed state.} \end{aligned} \tag{7}$$

Proof. We have that $\langle w_{ij} \rangle(r) = \rho_{ij}(r,r)$. In the case of a pure state, $\rho_{ij}(x,y) = \psi_i(x)\overline{\psi_j(y)}$, with $(\psi_1, \psi_2) \in \mathcal{H}$. Thus, the first of (7) follows from

$$\langle w_0 \rangle^2(r) - \left(\langle w_1 \rangle^2 + \langle w_2 \rangle^2 + \langle w_3 \rangle^2 \right)(r) = \det\left(\psi_i(r)\overline{\psi_j(r)} \right) = 0. \tag{8}$$

The mixed states have the form $\boldsymbol{\rho} = \sum_{k=1}^{\infty} \lambda_k \boldsymbol{\rho}_k$, where $\sum_{k=1}^{\infty} \lambda_k = 1$, $\lambda_k \geq 0$ and each $\boldsymbol{\rho}_k$ is a pure-state density matrix as above. By using (8) and the fact that $\det\,(tA + (1-t)B) \geq 0$ if $A \geq 0$, $B \geq 0$ and $t \in [0,1]$, we can inductively prove the second of (7) for a mixed state of the form $\boldsymbol{\rho} = \sum_{k=1}^{N} \lambda_k \boldsymbol{\rho}_k$. The general result follows by taking the limit $N \to \infty$. □

It is worth to remark that (7) are the same equations obeyed by the Stokes parameters describing a polarized light beam.[10]

Now, let A be a self adjoint operator acting on $\mathcal{H}$ (representing therefore a physical observable of our system) of the form

$$A = \boldsymbol{a}^{op} = \sum_{k=0}^{3} a_k^{op}\, \boldsymbol{\sigma}_k. \tag{9}$$

Here a_k^{op} denotes the Weyl quantization[5] of the symbol $a_k = a_k(r,p)$ (for each fixed k, a_k^{op} is an operator acting in $L^2(\mathbb{R}^3,\mathbb{C})$) and $\boldsymbol{a}^{op}$ is the corresponding matrix-valued symbol. If w_k are the Wigner functions associated to the density operator S as above, then it can be proved that[a]

$$\frac{1}{2}\ \mathrm{Tr}\,(SA) = \sum_{k=0}^{3} \int_{\mathbb{R}^6} a_k(r,p)\, w_k(r,p)\, dr\, dp. \tag{10}$$

Eq. (10) relates the expected value $\mathrm{Tr}(SA)$ of the observable A in the mixed state S with a "quasi-classical" expression involving the symbols a_k and the Wigner functions w_k. Note, in particular, that w_0 carries the information relevant to purely non-spinorial observables (e.g. position and momentum).

3. Application to the two-band k·p Hamiltonian

Using Pauli matrices, the two-band k·p Hamiltonian (3) can be written

$$H_{\mathrm{kp}} = \left(-\frac{\hbar^2}{2m}\,\Delta + V\right)\boldsymbol{\sigma}_0 - i\hbar\,\alpha\cdot\nabla\,\boldsymbol{\sigma}_2 + g\,\boldsymbol{\sigma}_3, \tag{11}$$

where we put $\alpha := \hbar K/m$ and $g := E_g/2$ for brevity. Note that $H_{\mathrm{kp}} = \boldsymbol{h}^{op}$, where the matrix-valued symbol $\boldsymbol{h}$ is given by

$$\boldsymbol{h}(r,p) = h_0(r,p)\,\boldsymbol{\sigma}_0 + \alpha\cdot p\ \boldsymbol{\sigma}_2 + g\,\boldsymbol{\sigma}_3 \tag{12}$$

and $h_0(r,p) := \frac{p^2}{2m} + V(r)$. The "free" k·p Hamiltonian (i.e. with $V = 0$) has a dispersion relation given by the eigenvalues of (11) with $V = 0$:

$$E_{\mathrm{c}}(p) = \frac{p^2}{2m} + \sqrt{(\alpha\cdot p)^2 + g^2}, \qquad E_{\mathrm{v}}(p) = \frac{p^2}{2m} - \sqrt{(\alpha\cdot p)^2 + g^2}, \tag{13}$$

(see Fig. 1). Two (non unitary) eigenvectors are

$$\psi_{\mathrm{c}}(p) = \begin{pmatrix} i\,\alpha\cdot p \\ g - \sqrt{(\alpha\cdot p)^2 + g^2} \end{pmatrix}, \qquad \psi_{\mathrm{v}}(p) = \begin{pmatrix} g - \sqrt{(\alpha\cdot p)^2 + g^2} \\ i\,\alpha\cdot p \end{pmatrix},$$

[a] Note that we denoted with "tr" the trace of a 2×2 complex matrix and with "Tr" trace of an operator acting on $\mathcal{H}$.

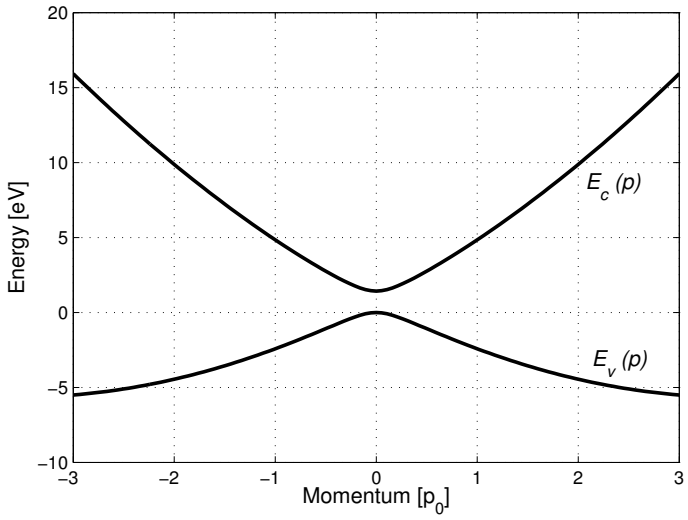

Figure 1. Plot of the energy eigenvalues $E_{\rm c}(p)$ and $E_{\rm v}(p)$ given by (13). Here the momentum variable p is assumed to be scalar. The energy unit is the electron Volt and the momentum unit is $p_0 = 3.8 \times 10^{-25}\,\mathrm{Kg\,m/sec}$. For the crystal parameters we used the values $E_g = 1.42\,\mathrm{eV}$ and $K = 1.3 \times 10^{10}\,\mathrm{m}^{-1}$, corresponding to the Γ-point of GaAs (the values are taken from Refs. 11 and 12).

from which we can compute the eigenprojections

$$\boldsymbol{\pi}_{\rm c}(p) = \frac{\psi_{\rm c}(p) \otimes \overline{\psi_{\rm c}(p)}}{|\psi_{\rm c}(p)|^2}, \qquad \boldsymbol{\pi}_{\rm v}(p) = \frac{\psi_{\rm v}(p) \otimes \overline{\psi_{\rm v}(p)}}{|\psi_{\rm v}(p)|^2},$$

so that the k·p symbol (12) can be written

$$\boldsymbol{h}(r,p) = E_{\rm c}(p)\,\boldsymbol{\pi}_{\rm c}(p) + E_{\rm v}(p)\,\boldsymbol{\pi}_{\rm v}(p) + V(r)\boldsymbol{\sigma}_0. \tag{14}$$

Carrying out the computations explicitly, we get

$$\boldsymbol{\pi}_{\rm c}(p) = \frac{1}{2}\boldsymbol{\sigma}_0 + \frac{\alpha\cdot p}{2\sqrt{(\alpha\cdot p)^2+g^2}}\boldsymbol{\sigma}_2 + \frac{g}{2\sqrt{(\alpha\cdot p)^2+g^2}}\boldsymbol{\sigma}_3,$$
$$\boldsymbol{\pi}_{\rm v}(p) = \frac{1}{2}\boldsymbol{\sigma}_0 - \frac{\alpha\cdot p}{2\sqrt{(\alpha\cdot p)^2+g^2}}\boldsymbol{\sigma}_2 - \frac{g}{2\sqrt{(\alpha\cdot p)^2+g^2}}\boldsymbol{\sigma}_3.$$

Introducing the vectors

$$\vec{B}(p) := (0,\, \alpha\cdot p,\, g), \qquad \vec{n}(p) := \frac{\vec{B}(p)}{|\vec{B}(p)|}, \qquad \vec{\boldsymbol{\sigma}} := (\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3) \tag{15}$$

the preceding expressions can be rewritten in the concise form

$$\boldsymbol{\pi}_{\rm c}(p) = \frac{1}{2}\,\boldsymbol{\sigma}_0 + \frac{1}{2}\,\vec{n}(p)\cdot\vec{\boldsymbol{\sigma}}, \qquad \boldsymbol{\pi}_{\rm v}(p) = \frac{1}{2}\,\boldsymbol{\sigma}_0 - \frac{1}{2}\,\vec{n}(p)\cdot\vec{\boldsymbol{\sigma}} \tag{16}$$

and the symbol $\boldsymbol{h}(r,p)$ in the following "spin-like" form:

$$\boldsymbol{h}(r,p) = h_0(r,p)\,\boldsymbol{\sigma}_0 + \vec{B}(p)\cdot\vec{\boldsymbol{\sigma}}. \tag{17}$$

The operators $\boldsymbol{\pi}_{\rm c}^{op}$ and $\boldsymbol{\pi}_{\rm v}^{op}$ (acting on $\mathcal{H}$) are the projections on the two band-subspaces of the free k·p Hamiltonian (note that they are *not* spectral projection for the full k·p Hamiltonian, i.e. with $V \neq 0$). Let us now consider the *band-index* operator $\boldsymbol{b}^{op}$ defined by the symbol

$$\boldsymbol{b}(p) := \boldsymbol{\pi}_{\rm c}(p) - \boldsymbol{\pi}_{\rm v}(p) = \vec{n}(p)\cdot\vec{\boldsymbol{\sigma}} \tag{18}$$

Clearly, $\boldsymbol{b}^{op}$ has eigenvalues 1 (for electrons in the conduction band) and -1 (for electrons in the valence band). Note that the band-index operator $\boldsymbol{b}^{op}$ has the form (9). Thus, from (18) and (10) we have that the expected value of the band index, in the mixed state described by the four Wigner functions w_k of Sec. 2, is given by

$$\frac{1}{2}\,\mathrm{Tr}\,(S\boldsymbol{b}^{op}) = \sum_{k=0}^{3}\int_{\mathbb{R}^6} \vec{n}(p)\cdot\vec{w}(r,p)\,dr\,dp, \tag{19}$$

where we put $\vec{w} = (w_1, w_2, w_3)$. This equation attaches a physical meaning to the "spinorial part" $\vec{w}$ of the Wigner functions defined in the previous section. Note that we can interpret the function $\vec{n}(p)\cdot\vec{w}(r,p)$ as a "band-index density in phase-space".

4. The k·p dynamics of Wigner functions

The evolution equation for the Wigner functions $w_k = w_k(t)$ is deduced from the evolution equation for the corresponding density operator $S(t)$, i.e, from the quantum Liouville equation

$$i\hbar\,\partial_t\,S(t) = [H_{\rm kp}, S(t)]\,, \tag{20}$$

where $[A,B] := AB - BA$, as usual. There is no room here to track all the computations that lead from (20) to the evolution equations for w_0 and $\vec{w} = (w_1, w_2, w_3)$. So, let us just show the final result, which reads as follows:

$$(\partial_t + v\cdot\nabla_r + \Theta_V)\,w_0 = -\nabla_r\cdot B'\,\vec{w} \tag{21a}$$

$$(\partial_t + v\cdot\nabla_r + \Theta_V)\,\vec{w} = \frac{2}{\hbar}\,\vec{B}\wedge\vec{w} - \nabla_r\cdot B'\,w_0 \tag{21b}$$

where $v := p/m$ and B' is the matrix $(\partial B_i/\partial p_j)$. At the right-hand sides of Eqs. (21) we just find the standard Wigner-equation operator[3] $v \cdot \nabla_r + \Theta_V$, where Θ_V is the pseudo-differential operator[5]

$$\Theta_V = \frac{i}{\hbar}\Big[V\Big(r + \frac{i\hbar}{2}\nabla_p\Big) - V\left(r - \frac{i\hbar}{2}\nabla_p\right)\Big], \tag{22}$$

with

$$[f(r, -i\hbar\nabla_p)u]\,(r,p) := \frac{1}{(2\pi\hbar)^3}\int_{\mathbb{R}^6} \mathrm{e}^{i(p-p')\cdot\xi/\hbar}\, f(r,\xi)\, u(r,p')\, d\xi\, dp'.$$

The first term at the right-hand side of Eq. (21b) generates a precession of $\vec{w}$ around the vector $\frac{2}{\hbar}\vec{B}$, where we recall that $\vec{B} = \vec{B}(p) = (0,\, \alpha\cdot p,\, g)$. The last terms of Eqs. (21) couple w_0 with $\vec{w}$. Since $\nabla_p \vec{B} = (0, \alpha, 0)$, i.e.

$$B' = \begin{pmatrix} 0 & 0 & 0 \\ \alpha_1 & \alpha_2 & \alpha_3 \\ 0 & 0 & 0 \end{pmatrix},$$

then we simply have $\nabla_r \cdot B'\,\vec{w} = \alpha \cdot \nabla_r w_2$ and $\nabla_r \cdot B'\, w_0 = \alpha \cdot \nabla_r (0, w_0, 0)$. Note, therefore, that the direct coupling takes place only through the second component w_2 of $\vec{w}$. Written component-wise, Eqs. (21) read as follows:

$$\begin{cases} \big(\partial_t + v\cdot\nabla_r + \Theta_V\big) w_0 = -\alpha\cdot\nabla_r\, w_2 \\ \big(\partial_t + v\cdot\nabla_r + \Theta_V\big) w_1 = -\dfrac{2g}{\hbar}\, w_2 + \dfrac{2}{\hbar}\,\alpha\cdot p\, w_3 \\ \big(\partial_t + v\cdot\nabla_r + \Theta_V\big) w_2 = -\alpha\cdot\nabla_r\, w_0 + \dfrac{2g}{\hbar}\, w_1 \\ \big(\partial_t + v\cdot\nabla_r + \Theta_V\big) w_3 = -\dfrac{2}{\hbar}\,\alpha\cdot p\, w_1. \end{cases} \tag{23}$$

If we now assume $V = 0$ and $g = 0$, then the system (23) take the simple form

$$\begin{cases} \big(\partial_t + v\cdot\nabla_r\big) w_0 = -\alpha\cdot\nabla_r\, w_2 \\ \big(\partial_t + v\cdot\nabla_r\big) w_1 = \dfrac{2}{\hbar}\,\alpha\cdot p\, w_3 \\ \big(\partial_t + v\cdot\nabla_r\big) w_2 = -\alpha\cdot\nabla_r\, w_0 \\ \big(\partial_t + v\cdot\nabla_r\big) w_3 = -\dfrac{2}{\hbar}\,\alpha\cdot p\, w_1. \end{cases} \tag{24}$$

Note that the vanishing band-gap, $g = 0$, makes w_0 and w_2 decoupled from w_1 and w_3. The system for w_0 and w_2 is a couple of transport equations

which can be easily solved; the general solution is

$$\begin{aligned} w_0(r,p,t) &= \frac{1}{2}\left[(w_0^0+w_2^0)(r-v_{\rm c}t,p)+(w_0^0-w_2^0)(r-v_{\rm v}t,p)\right], \\ w_2(r,p,t) &= \frac{1}{2}\left[(w_0^0+w_2^0)(r-v_{\rm c}t,p)-(w_0^0-w_2^0)(r-v_{\rm v}t,p)\right], \end{aligned} \tag{25}$$

where w_0^0, w_2^0 are arbitrary initial data for w_0, w_2 and we put

$$v_{\rm c} := v+\alpha = \frac{p}{m}+\alpha, \qquad v_{\rm v} := v-\alpha = \frac{p}{m}-\alpha.$$

Thus, we can observe that the initial Wigner functions are split into two packets which propagate with different p-dependent velocities, $v_{\rm c}$ and $v_{\rm v}$. This is due to the fact that the electron is, at each time, in a superposition of two energy-band states (valence and conduction) and the two bands have different dispersion relations, Eq. (13), i.e. two different group velocities. Note that in the simple case we are considering, i.e. $g=0$, the band-index density function is simply w_2 (in fact $\vec{n}=(0,1,0)$); thus w_2 represents the "presence" of the electron in conduction ($w_2 \geq 0$) and valence ($w_2 \leq 0$) bands.

If $g \neq 0$, the dynamics is more complicated and Eqs. (23) cannot be solved explicitly. In Figure 2 we show an example in dimension 1. We solved numerically Eqs. (23), with $V=0$, supplying it with the initial datum

$$\begin{aligned} w_0^0(r,p) &= \frac{1}{2\pi\Delta_r\Delta_p}\,\exp\left(-\frac{r^2}{2\Delta_r^2}-\frac{p^2}{2\Delta_p^2}\right), \\ w_1^0(r,p) &= w_2^0(r,p) = w_3^0(r,p) = 0, \end{aligned} \tag{26}$$

with $\Delta_r\Delta_p = \hbar/2$. This represents a mixed state (recall Proposition 2.1) consisting of a Gaussian wave packet centered in the origin of phase-space and equally distributed between the two bands (note, in fact, that the band-index density vanishes everywhere). The four figures are contour plots in phase-space (the level sets being logarithmically spaced) of the pseudo-distribution $w_0(r,p,t)$ at successive values of t. The first plot is just the initial datum. In the second plot the solution appears to be quite similar to the $g=0$ case, Eqs. (25): the conduction-part and the valence-part of the packet evolve according to its own dispersion relation (13). In the last two plots more complicated patterns appear, due to interference effects between the c-part and the v-part of the packet. The continuous line on the left-hand side of each plot represents the (half) local position density $\langle w_0\rangle(r,t) = \int_{-\infty}^{+\infty} w_0(r,p,t)\,dp$ (see Eq. (10)).

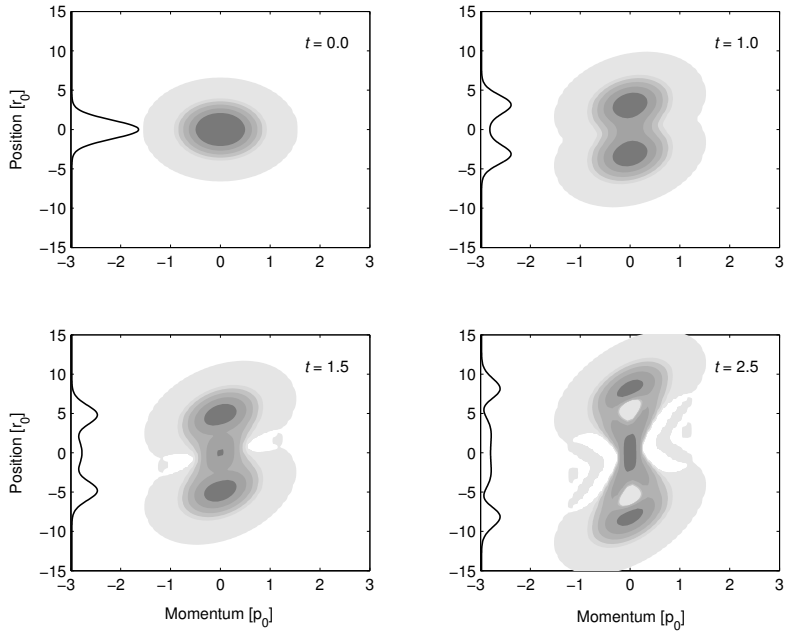

Figure 2. Evolution of the Gaussian wave-packet (26). The pseudo-distribution in phase-space w_0 is represented by the contour plots while the position density $\langle w_0 \rangle$, obtained by integrating w_0 with respect to p, is represented by the continuous lines at the left-hand side of each figure. The value of crystal parameters E_g and K, as well as the momentum unit p_0, are the same of Fig. 1. The length and time units are, respectively, $r_0 = 4.2 \times 10^{-10}$ m and 10^{-15} sec.

5. Balance equations

The pseudo-differential operator (22) can be formally expanded in a Taylor series of odd powers:

$$\Theta_V = -\sum_{|k| \text{ odd}} \left(\frac{i\hbar}{2}\right)^{|k|-1} \frac{\nabla_r^k V(r)}{k!} \nabla_p^k,$$

where we used the standard multi-index notations: $k := (k_1, k_2, k_3)$, $|k| := k_1+k_2+k_3$, $k! := k_1!\, k_2!\, k_3!$. Thus, for any given multi-index $s = (s_1, s_2, s_3)$, integration by parts yields

$$\int p^s\, \Theta_V\, u(r,p)\, dp = \sum_{|k| \text{ odd}}^{k \le s} \left(\frac{i\hbar}{2}\right)^{|k|-1} \frac{\nabla_r^k V(r)}{k!} \int p^{s-k} u(r,p)\, dp, \qquad (27)$$

where $k \leq s$ means $k_i \leq s_i$ for $i = 1, 2, 3$ (here and in the remainder of the paper the integrations are always intended to be over $p \in \mathbb{R}^3$).

Let now $(f_0, \vec{f})$ be a $\mathbb{R}^4$-valued function defined on phase-space. If we multiply Eq. (21a) by f_0, Eq. (21b) by $\vec{f}$ and add the resulting equations together, we obtain

$$\partial_t \left(f_0 w_0 + \vec{f} \cdot \vec{w} \right) + \nabla_r \cdot v \left(f_0 w_0 + \vec{f} \cdot \vec{w} \right) + \nabla_r \cdot B' \left(\vec{f} w_0 + f_0 \vec{w} \right) + f_0 \, \Theta_V w_0 + \vec{f} \cdot \Theta_V \vec{w} = \frac{2}{\hbar} \, \vec{f} \cdot \vec{B} \wedge \vec{w}. \quad (28)$$

By using (27) and (28), it is easy to deduce balance laws for the local densities of physical quantities carried by our system (recall Eq. (10)).

By substituting $(1, \vec{0})$ for $(f_0, \vec{f})$ in Eq. (28), and integrating with respect to p, we see from (27) that the potential terms vanish and obtain the continuity equation

$$\partial_t \, \rho + \nabla_r \cdot \vec{j} = 0, \quad (29a)$$

where $\rho := \langle w_0 \rangle = \int w_0 \, dp$ is (half) the position density and the current $\vec{j}$ is given by

$$\vec{j} := \int (v \, w_0 + B' \vec{w}) \, dp = \int (v \, w_0 + \alpha \, w_2) \, dp. \quad (29b)$$

Note that the current $\vec{j}$ is determined by a standard term $\int v \, w_0 \, dp$ and by a spinorial component $\alpha \int w_2 \, dp$, which is a correction that accounts for the different velocities of the c-part and the v-part of the electron.

From (17) we have that the observable "pseudo-kinetic energy", i.e. the non-potential part of energy, corresponds to the symbol $(f_0, \vec{f}) := (p^2/2m, \vec{B}(p))$. The (half) pseudo-kinetic energy density is, therefore, given by

$$\rho_E(r, t) := \int \left[\frac{p^2}{2m} \, w_0(r, p, t) + \vec{B}(p) \cdot \vec{w}(r, p, t) \right] dp \quad (30)$$

If we substitute $(p^2/2m, \vec{B}(p))$ for $(f_0, \vec{f})$ into (28), integrate with respect to p and observe that Eq. (27) yields

$$\int \frac{p^2}{2m} \, \Theta_V w_0 \, dp = \nabla_r V(r) \cdot \int \frac{p}{m} \, w_0 \, dp$$

$$\int \vec{B} \cdot \Theta_V \vec{w} \, dp = \nabla_r V(r) \cdot \int B' \vec{w} \, dp,$$

then we obtain the following balance law for ρ_E:

$$\partial_t \rho_E + \nabla_r \cdot \vec{j}_E = \vec{F} \cdot \vec{j}, \tag{31a}$$

where $\vec{F}(r) := -\nabla_r V(r)$ is the force field, $\vec{j}$ is given by (29b) and the pseudo-kinetic energy current $\vec{j}_E$ is given by

$$\vec{j}_E := \int v \left(\frac{p^2}{2m} w_0 + \vec{B} \cdot \vec{w} \right) dp + \int B' \left(\frac{p^2}{2m} \vec{w} + \vec{B} w_0 \right) dp. \tag{31b}$$

Note that Eq. (31a) has the familiar form of energy-balance laws: the change of energy density is due to the local energy flow $\nabla_r \cdot \vec{j}_E$ as well as to a "Joule heating" term $\vec{F} \cdot \vec{j}$.

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