Diffusive Limit of the Two-Band k·p Model for Semiconductors

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Abstract We derive semiclassical diffusive equations for the densities of electrons in the two energy bands of a semiconductor, as described by a k·p Hamiltonian. The derivation starts from a quantum kinetic (Wigner) description and resorts to the Chapman-Enskog method as well as to the quantum version of the minimum entropy principle. Four different regimes are investigated, according to different scalings of the k·p band-coupling and band-gap parameters with respect to the scaled Planck constant.

Keywords Quantum drift-diffusion · k·p model · Quantum entropy principle

1 Introduction

The origin of Quantum Fluid Dynamics (QFD) dates back to 1926 [26] when E. Madelung realized that Schrödinger equation admits a fluid-dynamic form which is formally identical to a pressureless Euler system with a quantum correction (of order $\hbar^2$) involving what nowadays is known as "Bohm potential" [5, 6]. Since the first half of nineties [16] the interest in QFD has been rapidly increasing because of applications to semiconductor devices modeling (see Ref. [19] and references therein). Indeed, QFD-like models are the meeting point between two fundamental requirements: the incorporation of quantum effects (which in modern nanoscale devices are no longer negligible and may dominate the behavior of the device) and the preference for fluid-dynamic descriptions (hydrodynamics, energy transport, drift-diffusion, etc.) which are relatively simple, flexible and cheap from the computational point of view.

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There are basically two roads to QFD. The first is the one followed by Madelung and consists in inserting the WKB Ansatz $\psi = \sqrt{n}\, e^{iS/\hbar}$ into Schrödinger equation. This yields relations between the density n and the current $J = n\nabla S$. The second road starts from the kinetic-like formulation of quantum mechanics due to Wigner [32, 36, 39] and, in much the same way as one goes from classical kinetic to classical fluid equations, consists in writing equations for the moments of the Wigner functions (pseudo-distributions on phase-space):

$$n(x) = \int w(x, p)\, dp, \qquad J(x) = \int p\, w(x, p)\, dp.$$

Both roads are equivalent [17, 18] but the use of Wigner functions is often of great interest because it allows one to stick to the classical case.

While Madelung equations (which hold for a pure quantum state) are formally closed and equivalent to the Schrödinger equation [17], in the case of mixed (statistical) states the equations for n and J are not closed, i.e. they contain terms depending of higher-order moments. The problem of the closure of mixed-state quantum hydrodynamic equations has been set on a solid basis by Degond and Ringhofer [13] who extended to the quantum case Levermore's entropy minimization principle [25]. This principle, which is intimately connected with maximum likelihood principle in statistics, stipulates that an observed set M of macroscopic moments is the manifestation of an underlying local equilibrium state which, among all states having the same macroscopic moments M, is the minimizer of a suitable entropy functional $\mathcal{A}$. This implies that the state to be used for the closure of fluid-dynamic equations for a certain set of moments M satisfies a constrained minimization problem:

Find a minimizer of $\mathcal{A}$ under the constraint that the moments M are given.

In the quantum case, once such a local equilibrium state has been found, one can expand it semiclassically (i.e. in powers of $\hbar$) in order to obtain quantum corrections to fluid equations up to the desired order (usually $\hbar^2$, which is sufficient for including Bohm-like terms). Many subsequent works use the quantum version of the entropy minimization principle in order to obtain QFD models of various kind (hydrodynamics, energy transport, SHE-model, drift-diffusion) [4, 8–12, 20, 21].

All the works quoted above, as well as most of works appeared in the literature, consider the case of a scalar Hamiltonian of the form $p^2/2m + V(x)$. To our knowledge, however, derivations of QHD equations for *spinorial* systems, i.e. systems having additional, discrete, degrees of freedom, are still almost absent in the literature and the few examples we are aware of [2, 7, 27, 34, 40] do not exploit the quantum entropy minimization principle.

In the present paper we study the application of Degond and Ringhofer's technique to a (pseudo)spinorial case of interest in semiconductor physics, namely the two-band "k·p" Hamiltonian

$$H = \begin{pmatrix} -\frac{\hbar^2}{2m}\Delta + E_g/2 & -\frac{\hbar^2}{m}K\cdot\nabla \\ \frac{\hbar^2}{m}K\cdot\nabla & -\frac{\hbar^2}{2m}\Delta - E_g/2 \end{pmatrix}$$

which describes electrons in a periodic potential with two available energy bands [23, 35]. The band-gap E_g and the coupling vector $K = (K_1, K_2, K_3)$ will be referred to as "crystal parameters" or "band parameters". The k·p Hamiltonian acts on wavefunctions in $L^2(\mathbb{R}^3, \mathbb{C}^2)$ and, therefore, the system has a spin-like degree of freedom, called *pseudospin*. The meaning of such pseudospin is related to the energy bands, as it will be explained in Sect. 2. Our ultimate goal is the formal derivation of diffusive semiclassical equations for the densities, n_+ and n_-, of the electrons in the two bands.

To this aim, once the kinetic (Wigner) equations for the k·p system have been written, interaction effects are introduced under the form of a BGK-like term making the system relax to a local equilibrium state. The band densities n_+ and n_- are then suitably defined and the local equilibrium state is assumed to be given by the quantum entropy minimization principle, under the constraint of given moments n_+ and n_-. This is equivalent to assuming that the BGK collisions do not allow band-crossings. Band transitions, therefore, are exclusively due to external potentials. Here by "external potentials" we mean any electrostatic potential different from the one generated by the semiconductor ion lattice and may comprise, therefore, external bias, self-consistent Coulomb potentials, heterostructure potentials etc. Such field-mediated band transitions are known as "Zener tunneling" [22] and are of the utmost importance for the so-called interband semiconductor devices [31, 37]. Of course, band-crossing collisions can always be added to the model, if desired.

After writing the Wigner-BGK equation in terms of dimensionless variables, two parameters appear which are assumed to be small: a diffusive parameter τ (the scaled typical collision time) and a semiclassical parameter ϵ (the scaled Planck constant). Also the dimensionless band parameters will appear in the equations, namely the scaled coupling vector $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ and the scaled (half) band-gap γ. First, we look for the formal quantum diffusive limit ($\tau \to 0$, $\epsilon \sim 1$) by applying to Wigner-BGK equations the Chapman-Enskog method at first order. The result is summarized in Theorem 4.1 and consists of two coupled equations for n_+ and n_- (see (4.9) or the equivalent, but more explicit, (4.14)). However, these equations are only of theoretical interest, since they are rather involved, especially because of the complicated dependence of the local equilibrium g on the moments n_+ and n_-, as resulting from the constrained entropy minimization. Therefore, our next step is to take the semiclassical limit $\epsilon \to 0$ of the quantum diffusive equations (4.14). To this aim we first have to expand the constrained entropy minimizer g up to first order in ϵ, which can be done explicitly by using Moyal calculus (see Theorem 5.2). Then, the formal semiclassical limit of the diffusive equations is computed in four cases, according to different scalings of the band parameters α and γ with respect to ϵ, namely ($\alpha \sim 1$, $\gamma \sim 1$), ($\alpha \sim \epsilon$, $\gamma \sim \epsilon$), ($\alpha \sim \epsilon$, $\gamma \sim 1$), ($\alpha \sim 1$, $\gamma \sim \epsilon$) (see Theorems 6.1–6.4). In the first case, representing strong influence of the crystal lattice, we obtain a system of drift-diffusion-like equations with complicated effective-mass effects and nonlinear interband coupling terms, see (6.13). The nonlinear coupling comes from the first-order quantum correction to the classical equilibrium distribution, which is a remarkable feature of the spinorial case because, instead, first-order corrections always vanish for scalar Hamiltonians [36]. The second, opposite, case is also interesting since it results in a system of standard (i.e. with parabolic dispersion relations) drift-diffusion equations (6.18) with a linear, field-dependent, coupling term which induces a relaxation of the band polarity. In the third case, where the coupling vector α vanishes and the bands remain separated by a band-gap 2γ, the semiclassical limit is trivial, consisting of two decoupled parabolic drift-diffusion equations (6.20). The last case (vanishing band-gap) produces in the limit a band-crossing, and therefore a singularity, along the plane $\alpha \cdot p = 0$. We shall call it a "Dirac plane" because of the evident analogy with Dirac points in the spectrum of relativistic massless particles [33] as well as of materials such as graphene [15, 24]. The singularity prevents the diffusive equations from having a finite limit for $\epsilon \to 0$. However, we show that changing the definition of energy bands from "upper/lower" to "pseudospin up/down" yields decoupled drift-diffusion equations (6.24) for the populations of such newly-defined bands. This fact can be properly interpreted in terms of pseudospin conservation (see Remark 6.3).

Note that in the present paper we do not consider semiclassical corrections of order ϵ^2 and, consequently, Bohm-like terms are missing. A two-band drift-diffusion model for a

spin-orbit Hamiltonian, based on the quantum minimum entropy principle, has been recently obtained in Ref. [3], with the inclusion of ϵ^2 terms. However, although spin densities have a simpler structure than k·p band densities (basically, $w_{\uparrow\downarrow} = w_1 \pm w_3$ substitutes definition (4.2)), the ϵ^2 corrections turn out to be very complicated. This fact suggested us not to introduce further complications in the present paper and to postpone the computation of higher-order corrections for the k·p case to future works.

The outline of the paper is as follows. In Sect. 2 we introduce the k·p Hamiltonian and related concepts such as energy bands, pseudospin and band projections. In Sect. 3 we introduce the kinetic description of the system, define the local band-densities n_+ and n_-, and write down the Wigner-BGK (WBGK) equations. The scaling of the WBGK equations, with the introduction of the diffusive and semiclassical parameters, is performed in Sect. 3.2. Section 4 is devoted to the derivation of the quantum diffusive equations by applying the Chapman-Enskog method (Theorem 4.1). The characterization of the local equilibrium state g as the solution of the constrained entropy-minimization problem is given in Sect. 5.1. The proof of the characterization theorem (Theorem 5.1) is postponend to the Appendix. In Sect. 5.2 the semigroup equation for g is written, which is used in next Sect. 5.3 to explicitly compute the first two terms of the semiclassical expansion of g (Theorem 5.2). These computations are then used in Sect. 6 to study the semiclassical limits of the quantum diffusive model in the four cases mentioned above (Theorems 6.1–6.4).

2 The k·p Model

The simplest possible description of an electron in a semiconductor crystal with two energy bands (e.g. "valence" and "conduction") is obtained from a periodic Hamiltonian by means of the k·p method [23, 35] and consists of a 2×2 Hamiltonian of the following form:

$$H = \begin{pmatrix} -\frac{\hbar^2}{2m}\Delta + E_g/2 & -\frac{\hbar^2}{m}K \cdot \nabla \\ \frac{\hbar^2}{m}K \cdot \nabla & -\frac{\hbar^2}{2m}\Delta - E_g/2 \end{pmatrix}. \tag{2.1}$$

Here, E_g is the band-gap and $K = (K_1, K_2, K_3)$ is the matrix element of the gradient operator between the Bloch functions $u_\pm$ of the upper (+) and lower (−) bands, evaluated at zero pseudo-momentum:

$$K = \int_{lattice\ cell} \overline{u}_+(x) \nabla u_-(x)\, dx.$$

The k·p model has to be completed by adding an "external" potential term qV (where $q > 0$ denotes the elementary charge), accounting for all electric fields except the crystal one. The electric potential $V(x)$ can be either fixed or self-consistently given by a Poisson equation.

The "free" k·p Hamiltonian H is the quantization of the classical matrix-valued symbol

$$h(p) = \begin{pmatrix} \frac{p^2}{2m} + E_g/2 & -i\frac{\hbar}{m}K \cdot p \\ i\frac{\hbar}{m}K \cdot p & \frac{p^2}{2m} - E_g/2 \end{pmatrix}. \tag{2.2}$$

It will be convenient to decompose any 2×2 complex matrix in the basis of Pauli matrices

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

(the coefficients of the decomposition will be real if the matrix is hermitian). The operators σ_1, σ_2, σ_3 are called "pseudospin components" in this context. Putting

$$\alpha = (\alpha_1, \alpha_2, \alpha_3) := \frac{\hbar}{m} K \quad \text{and} \quad \gamma := E_g/2, \tag{2.3}$$

we can write

$$h(p) = \frac{p^2}{2m}\sigma_0 + \alpha \cdot p\sigma_2 + \gamma\sigma_3 = h_0(p)\sigma_0 + \vec{h}(p) \cdot \vec{\sigma}, \tag{2.4}$$

where

$$h_0(p) = \frac{p^2}{2m}, \qquad \vec{h}(p) = (0, \alpha \cdot p, \gamma),$$

and, as usual, $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is the formal vector of Pauli matrices.

Remark 2.1 Here and in the following we adopt the arrow notation for three-vectors, such as $\vec{h}(p)$, that are the (pseudo)spinorial part of the Pauli coefficients. Instead, we do not use the arrow notation for "cartesian" three-vectors such as x, p, K, α etc.

The dispersion relation for the free Hamiltonian H is easily obtained by computing the (p-dependent) eigencouples of the symbol $h(p)$. This yields the *energy bands*

$$E_\pm(p) = \frac{p^2}{2m} \pm \sqrt{(\alpha \cdot p)^2 + \gamma^2} = \frac{p^2}{2m} \pm |\vec{h}(p)| \tag{2.5}$$

and the corresponding normalized energy eigenvectors

$$\psi_\pm^p = \frac{1}{\sqrt{2(1 \pm v_3(p))}} \begin{pmatrix} v_3(p) \pm 1 \\ v_1(p) + i v_2(p) \end{pmatrix}, \tag{2.6}$$

where we have introduced

$$\vec{v}(p) = (v_1(p), v_2(p), v_3(p)) = \frac{\vec{h}(p)}{|\vec{h}(p)|} = \frac{(0, \alpha \cdot p, \gamma)}{\sqrt{(\alpha \cdot p)^2 + \gamma^2}}. \tag{2.7}$$

The two eigenprojections $P_\pm(p)$, that we call *band-projections*, are therefore given by

$$P_\pm(p) = \psi_\pm^p \otimes \psi_\pm^p = \frac{1}{2}(\sigma_0 \pm \vec{v}(p) \cdot \vec{\sigma}) \tag{2.8}$$

and we can clearly write

$$h(p) = E_+(p)P_+(p) + E_-(p)P_-(p). \tag{2.9}$$

Other interesting observables are the *band index*

$$B(p) = \vec{v}(p) \cdot \vec{\sigma}, \tag{2.10}$$

so that $P_\pm(p) = \frac{1}{2}(\sigma_0 \pm B(p))$, and the velocity vector operator

$$U(p) = \nabla_p h(p) = \begin{pmatrix} p/m & -i\alpha \\ i\alpha & p/m \end{pmatrix} = \frac{p}{m}\sigma_0 + \alpha\sigma_2. \tag{2.11}$$

Remark 2.2 Note that the eigenvectors of $U(p)$ are of the form

$$\varphi_{\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm i \end{pmatrix}, \tag{2.12}$$

with eigenvalues $p/m \pm \alpha$. Here, the subscripts $\pm$ do *not* correspond to the band indices unless $\vec{v}(p) = \vec{e}_2 = (0, 1, 0)$ (i.e. $\gamma = 0$). In other words, only in the case $\vec{v}(p) = \vec{e}_2$ the energy eigenstates are simultaneously velocity eigenstates (and, of course, eigenstates of the pseudospin σ_2).

Clearly, the corresponding operators $P_{\pm}$, B and U acting on the wavefunction space $L^2(\mathbb{R}^3, \mathbb{C}^2)$ are obtained from $P_{\pm}(p)$, $B(p)$ and $U(p)$ by the quantization rule $p \mapsto -i\hbar\nabla$. The corresponding (generalized) eigenstates are

$$\psi_{\pm}^p(x) = \psi_{\pm}^P e^{ip\cdot x/\hbar},$$

for h, $P_{\pm}$ and B, and

$$\varphi_{\pm}^p(x) = \varphi_{\pm} e^{ip\cdot x/\hbar}$$

for U, where $\psi_{\pm}^P$ and $\varphi_{\pm}$ are given by (2.6) and (2.12).

3 Wigner-BGK Equation for the k·p Model

In this section we introduce the kinetic description of the k·p system, which is based on the Wigner formulation of statistical quantum mechanics [36]. In such a framework, as we shall see, the definition of local densities and the introduction of relaxation-time collision operator are particularly straightforward.

3.1 Spinorial Wigner Functions

A mixed (statistical) quantum state for a system governed by the k·p Hamiltonian H is described by a density operator S, i.e. a bounded nonnegative operator, with unit trace, acting on $L^2(\mathbb{R}^3, \mathbb{C}^2)$. However, the statistical quantum mechanics has a "kinetic" formulation due to Wigner [32, 36, 39] which, because of its analogies with classical kinetic theory, is particularly suitable as a "mesoscopic" description leading, eventually, to fluid-dynamic equations for macroscopic averages [19]. The Wigner transform $w = w(x, p)$ of a (scalar) function $\rho = \rho(x, y)$ is

$$w(x, p) = (\mathcal{W}\rho)(x, p) = \int_{\mathbb{R}^3} \rho\left(x + \frac{\xi}{2}, x - \frac{\xi}{2}\right) e^{-ip\cdot\xi/\hbar} d\xi, \tag{3.1}$$

and its inverse is given by

$$\rho(x, y) = (\mathcal{W}^{-1}w)(x, y) = \frac{1}{(2\pi\hbar)^3} \int_{\mathbb{R}^3} w\left(\frac{x+y}{2}, p\right) e^{i(x-y)\cdot p/\hbar} dp. \tag{3.2}$$

The connection with mixed states arises from the fact that a (scalar) density operator S admits an integral representation

$$(S\psi)(x) = \int_{\mathbb{R}^3} \rho^S(x, y)\psi(x) \, dy$$

whose associated integral kernel ρ^S is the so-called density matrix. Therefore, we can associate to a mixed state, with density operator S, a Wigner function

$$w = \mathcal{W}\rho^S = \text{Op}_\hbar^{-1}(S),$$

which turns out to be real-valued. The notation $\text{Op}_\hbar^{-1}$ is due to the fact that $S \mapsto \rho^S \mapsto w$ is exactly the inverse of the Weyl quantization [14, 39] which associates a classical phase-space symbol $a(x, p)$ with the operator

$$[\text{Op}_\hbar(a)\psi](x) = \frac{1}{(2\pi\hbar)^3} \int_{\mathbb{R}^6} a\left(\frac{x+y}{2}, p\right)\psi(y)\, e^{i(x-y)\cdot p/\hbar}\, dy\, dp. \tag{3.3}$$

Note, in fact, that $\text{Op}_\hbar(a)$ is an integral operator with formal kernel $\mathcal{W}^{-1}a$.

In our "spinorial" case, the density operator S acts on $L^2(\mathbb{R}^3, \mathbb{C}^2)$ and then it has a 2×2 density matrix $\rho_{ij}^S(x, y)$. Thus, we can associate with S a 2×2 matrix of Wigner functions $w_{ij} = w_{ij}(x, p)$ given by

$$w_{ij} = \mathcal{W}\rho_{ij}^S = \text{Op}_\hbar^{-1}(S_{ij}) \tag{3.4}$$

or, briefly,

$$w = \mathcal{W}\rho^S = \text{Op}_\hbar^{-1}(S),$$

which turns out to be hermitian

$$\overline{w_{ij}(x, p)} = w_{ji}(x, p).$$

It will be convenient to consider the Pauli components of the Wigner matrix w, which are four real-valued functions on phase-space,

$$w = w_0\sigma_0 + \vec{w} \cdot \vec{\sigma}, \quad \vec{w} = (w_1, w_2, w_3).$$

In this way we have a very simple, and classical-fashioned, formula for the expected value of an observable A in the state S:

$$\frac{1}{2}\text{Tr}(SA) = \frac{1}{2}\text{Tr}(AS) = \sum_{k=0}^{3} \int_{\mathbb{R}^6} a_k(x, p)w_k(x, p)\, dx\, dp, \tag{3.5}$$

where $S = \sum_{k=0}^{3} \text{Op}_\hbar(w_k)\sigma_k$ and $A = \sum_{k=0}^{3} \text{Op}_\hbar(a_k)\sigma_k$. Such identity allows to consider the *local density* (or *moment*) of the observable A in the state S as

$$\frac{1}{2}\text{Tr}(SA \mid x) = \sum_{k=0}^{3} \int_{\mathbb{R}^3} a_k(x, p)w_k(x, p)\, dp. \tag{3.6}$$

In particular, we shall be interested in the *local band-densities* $n_\pm(x)$, that are the local densities of the band-projections $P_\pm$ defined in the previous section. Since Weyl quantization reduces to standard quantization for symbols depending only on p (and also for symbols depending only on x), from (2.8) we have $P_\pm = \frac{1}{2}(\sigma_0 \pm \text{Op}_\hbar(\vec{v}) \cdot \vec{\sigma})$ and then, according to (3.6), the local densities are given by

$$n_\pm(x) = \text{Tr}(SP_\pm \mid x) = \int_{\mathbb{R}^3} [w_0(x, p) \pm \vec{v}(p) \cdot \vec{w}(x, p)]dp. \tag{3.7}$$

3.2 Wigner-BGK Equations

Assume now that the dynamics of the time dependent mixed state $S(t)$ is given by the von Neumann equation (Schrödinger equation for mixed states)

$$i\hbar\partial_t S(t) = [H + qV\sigma_0, S(t)],$$

where H is the k·p Hamiltonian (2.1), $qV\sigma_0$ is the external field term and, as usual, $[A, B]$ denotes the commutator $AB - BA$. Then, using (3.1), it is not difficult to prove that the evolution equations for the corresponding time dependent Pauli-Wigner functions

$$w_k = w_k(t) = w_k(x, p, t), \qquad w(t) = \text{Op}_\hbar^{-1}(S(t)),$$

are the following:

$$\begin{cases} (\partial_t + \frac{p}{m} \cdot \nabla_x + q\Theta_\hbar[V])w_0 + \alpha \cdot \nabla_x w_2 = 0, \\ (\partial_t + \frac{p}{m} \cdot \nabla_x + q\Theta_\hbar[V])\vec{w} + \alpha \cdot \nabla_x w_0\,\vec{e}_2 - \frac{2}{\hbar}\vec{h}(p) \times \vec{w} = 0. \end{cases} \tag{3.8}$$

Here, $\vec{h}(p) = (0, \alpha \cdot p, \gamma)$, $\vec{e}_2 = (0, 1, 0)$ and $\Theta_\hbar[V]$ is the pseudo-differential operator

$$\Theta_\hbar[V] = \frac{i}{\hbar}\left[V\left(x + \frac{i\hbar}{2}\nabla_p\right) - V\left(x - \frac{i\hbar}{2}\nabla_p\right) \right], \tag{3.9}$$

that is, more explicitly,

$$\begin{aligned} &[\Theta_\hbar[V]w](x, p, t) \\ &= \frac{i}{\hbar}\int_{\mathbb{R}^6}\left[V\left(x + \frac{\xi}{2}\right) - V\left(x - \frac{\xi}{2}\right) \right] e^{i\xi \cdot (p'-p)/\hbar} w(x, p', t)\frac{d\xi\,dp'}{(2\pi\hbar)^3}. \end{aligned}$$

System (3.8) just describes a single-particle Hamiltonian dynamics. Since we are interested to the diffusive regime, collisional effects have to be inserted somehow. A simple model taking account of collisions, that force the system towards a local equilibrium, is obtained by adding relaxation-time terms of BGK (Bhatnaghar-Gross-Krook) type [1]

$$\begin{cases} (\partial_t + \frac{p}{m} \cdot \nabla_x + q\Theta_\hbar[V])w_0 + \alpha \cdot \nabla_x w_2 = \frac{g_0 - w_0}{\tau_c}, \\ (\partial_t + \frac{p}{m} \cdot \nabla_x + q\Theta_\hbar[V])\vec{w} + \alpha \cdot \nabla_x w_0\,\vec{e}_2 - \frac{2}{\hbar}\vec{h}(p) \times \vec{w} = \frac{\vec{g} - \vec{w}}{\tau_c}, \end{cases} \tag{3.10}$$

where τ_c is the relaxation time (which is assumed to be the same constant for all components) and $g = g_0\sigma_0 + \vec{g} \cdot \vec{\sigma}$ is a local-equilibrium Wigner matrix that will be specified later on. System (3.10) will be referred to as "Wigner-BGK" (WBGK) equations.

3.3 Scaling the WBGK Equations

In order to rewrite system (3.10) in scaled form, let us introduce the reference length x_0, time t_0, momentum p_0, potential V_0 and density N_0, and switch to dimensionless quantities:

$$x \to x_0 x, \qquad t \to t_0 t, \qquad p \to p_0 p, \qquad V \to V_0 V, \qquad w \to N_0 w, \qquad g \to N_0 g,$$

(for the sake of simplicity the new, dimensionless, variables are denoted by the same symbols as the old ones). After some algebra, (3.10) can be written in dimensionless form as

$$
\begin{cases}
(\frac{mx_0}{t_0 p_0}\partial_t + p \cdot \nabla_x + \frac{mqV_0}{p_0^2}\Theta_{\frac{\hbar}{x_0 p_0}}[V])w_0 + \frac{m}{p_0}\alpha \cdot \nabla_x w_2 = \frac{mx_0}{p_0 \tau_c}(g_0 - w_0), \\
(\frac{mx_0}{t_0 p_0}\partial_t + p \cdot \nabla_x + \frac{mqV_0}{p_0^2}\Theta_{\frac{\hbar}{x_0 p_0}}[V])\vec{w} + \frac{m}{p_0}\alpha \cdot \nabla_x w_0 \vec{e}_2 \\
\quad - \frac{2mx_0}{p_0 \hbar}\vec{h}(p_0 p) \times \vec{w} = \frac{mx_0}{p_0 \tau_c}(\vec{g} - \vec{w}).
\end{cases}
$$

Now let us make the following assumptions:

 (i) the momentum reference value p_0 is chosen as being the thermal one, $p_0 = \sqrt{mk_B T}$, where k_B is Boltzmann constant and T is the (constant) temperature of the thermal bath;
 (ii) the electric potential reference value V_0 is chosen such that $qV_0 = p_0^2/m = k_B T$, which amounts to assume that the potential energy is on the same scale as the typical kinetic energy of electrons;
(iii) the reference time t_0 is on the diffusive time scale.

The last assumption implies that, if we define the *diffusive parameter* τ as the scaled collision time

$$
\tau = \frac{p_0 \tau_c}{mx_0}, \tag{3.11}
$$

then, in order to have the time derivative multiplied by τ, we must choose t_0 such that $\frac{mx_0}{t_0 p_0} = \tau$, i.e.

$$
t_0 = \frac{m^2 x_0^2}{p_0^2 \tau_c} = \frac{mx_0^2}{k_B T \tau_c}. \tag{3.12}
$$

We also introduce the *semiclassical parameter* ϵ as the scaled Planck constant

$$
\epsilon = \frac{\hbar}{x_0 p_0}, \tag{3.13}
$$

and (without changing the symbols, for the sake of simplicity) redefine the scaled crystal parameters α and γ as

$$
\frac{m}{p_0}\alpha \to \alpha, \qquad \frac{m}{p_0^2}\gamma \to \gamma. \tag{3.14}
$$

All this considered, the dimensionless WBGK equations take the scaled form

$$
\begin{cases}
(\tau\partial_t + p \cdot \nabla_x + \Theta_\epsilon[V])w_0 + \alpha \cdot \nabla_x w_2 = \frac{g_0 - w_0}{\tau}, \\
(\tau\partial_t + p \cdot \nabla_x + \Theta_\epsilon[V])\vec{w} + \alpha \cdot \nabla_x w_0 \vec{e}_2 - \frac{2}{\epsilon}\vec{h}(p) \times \vec{w} = \frac{\vec{g} - \vec{w}}{\tau},
\end{cases} \tag{3.15}
$$

where $\vec{h}(p)$ keeps the form

$$
\vec{h}(p) = (0, \alpha \cdot p, \gamma) \tag{3.16}
$$

but now p, α, γ are the new scaled quantities.

Remark 3.1 Of course, one may obtain the same equations by starting from the scaled Hamiltonian

$$h(p) = \begin{pmatrix} \frac{1}{2}p^2 + \gamma & -i\alpha \cdot p \\ i\alpha \cdot p & \frac{1}{2}p^2 - \gamma \end{pmatrix}.$$

(obtained from the unscaled expression (2.2) dividing by the reference energy p_0^2/m) and using the scaled Weyl-Wigner correspondence:

$$\mathrm{Op}_{\frac{\hbar}{p_0 x_0}} = \mathrm{Op}_\epsilon.$$

4 Quantum Diffusive Limit

Our first goal is to derive a quantum diffusive model for the time dependent band densities $n_\pm(x, t)$, introduced in Sect. 3. We recall here their definition for a time dependent mixed state:

$$n_\pm(x, t) = \int_{\mathbb{R}^3} [w_0(x, p, t) \pm \vec{v}(p) \cdot \vec{w}(x, p, t)] dp. \tag{4.1}$$

Since we have adopted the same symbols for scaled and unscaled variable, this expression is the same in both cases. For later convenience we introduce the notations

$$w_\pm(x, p, t) := w_0(x, p, t) \pm \vec{v}(p) \cdot \vec{w}(x, p, t) \tag{4.2}$$

and, for any given $f = f(x, p, t)$,

$$\langle f \rangle(x, t) := \int_{\mathbb{R}^3} f(x, p, t) \, dp, \tag{4.3}$$

so that definition (4.1) can be simply written as

$$n_\pm = \langle w_\pm \rangle.$$

Quantum diffusive equations for $n_\pm$ can be derived by performing an asymptotic analysis, based on the Chapman-Enskog method, of (3.15) for the small parameter τ. To this aim we have to be more precise about the local equilibrium state $g = g_0\sigma_0 + \vec{g} \cdot \vec{\sigma}$ appearing in the WBGK equation (3.15). However, for the time being, we can postpone a detailed discussion about g to Sect. 5 and introduce just the properties that are needed here. Since in this work we are mainly interested in band-transitions induced by the electric field V (the so-called Zener tunneling [22]), then we assume that *collisions do not produce band-crossings*. Hence, the BGK operator must conserve the band densities n_+ and n_-, which leads to the fundamental moment constraints

$$\langle g_\pm \rangle = n_\pm = \langle w_\pm \rangle. \tag{4.4}$$

Of course, it is always possible to include band-crossing collisions in the model, which eventually lead to additional coupling terms in the diffusive equations, but this issue will not be discussed in the present paper.

In order to apply the Chapman-Enskog method, let us rewrite the scaled WBGK system (3.15) in compact form as follows:

$$\tau \partial_t w^\tau + T w^\tau = \frac{g[n^\tau] - w^\tau}{\tau}, \tag{4.5}$$

where, using Pauli components,

$$(Tw)_0 = (p \cdot \nabla_x + \Theta_\epsilon[V]) w_0 + \alpha \cdot \nabla_x w_2,$$
$$(\vec{T w}) = (p \cdot \nabla_x + \Theta_\epsilon[V]) \vec{w} + \alpha \cdot \nabla_x w_0 \, \vec{e}_2 - \frac{2}{\epsilon} \vec{h}(p) \times \vec{w}. \tag{4.6}$$

In (4.5) we added an index τ to stress the dependence of w on the diffusive parameter τ. Moreover, we introduced the notation $g[n^\tau]$ to stress the dependence of g on the couple of moments

$$n^\tau := (n_+^\tau, n_-^\tau) = (\langle w_+^\tau \rangle, \langle w_-^\tau \rangle) \tag{4.7}$$

of the unknown w^τ, as it implicitly results from the constraints (4.4).

Theorem 4.1 (Formal diffusive limit) *Assume that $n^\tau = (n_+^\tau, n_-^\tau)$ converges as $\tau \to 0$ to some limit couple of densities $n = (n_+, n_-)$, and assume that $g[n^\tau]$ is such that*

$$\langle (T g[n^\tau])_\pm \rangle = 0 \tag{4.8}$$

for all $\tau > 0$. Then $n_+(x, t)$ and $n_-(x, t)$ satisfy the evolution equation

$$\partial_t n_\pm = \langle (T T g[n])_\pm \rangle. \tag{4.9}$$

Proof First of all (assuming the map $n \mapsto g[n]$ to be continuous) we observe that passing to the limit for $\tau \to 0$ in (4.5) yields

$$w^\tau \to g[n],$$

which means that the 0-order approximation for w^τ is the local equilibrium relative to the limit moments. The Chapman-Enskog Ansatz reads as follows:

$$w^\tau = g[n^\tau] + \tau w^{(1)}, \tag{4.10}$$

where $w^{(1)}$ is, therefore, a perturbation of the local equilibrium state. By substituting (4.10) into the WBGK equation (4.5) we obtain

$$\tau \partial_t w^\tau + T g[n^\tau] + \tau T w^{(1)} = -w^{(1)}$$

which, for $\tau \to 0$, yields

$$w^{(1)} = -T g[n]. \tag{4.11}$$

Thus, by substituting again in the previous equation, we have

$$\tau \partial_t w^\tau + T g[n^\tau] - \tau T T g[n] = T g[n].$$

If we now take the moments $\langle (\cdot)_\pm \rangle$ of both sides of the latter equation, and use the constraints (4.4), we obtain

$$\tau \partial_t n_\pm + \langle (T g[n^\tau])_\pm \rangle - \tau \langle (T T g[n])_\pm \rangle = \langle (T g[n])_\pm \rangle.$$

Thus, by using assumption (4.8) (that continuity guarantees to hold also for $g[n]$), (4.9) follows. □

Remark 4.1 System (4.9) is the diffusive limit of the kinetic model (3.15). It is formally closed provided that g can actually be expressed as a function of n_+ and n_- by using the constraints (4.4). Moreover, g should satisfy condition (4.8). In Sect. 5 we shall prove that, if g is given by a minimum entropy principle, then it satisfies condition (4.8) (see Proposition 5.1) and, moreover, we shall write explicitly g as a function of n_+ and n_-, at least in the semiclassical approximation.

In view of the subsequent semiclassical analysis, let us end the section putting system (4.9) in a more explicit form. For the sake of brevity we simplify notations by defining

$$\Theta := \Theta_\epsilon[V], \qquad \partial_i := \frac{\partial}{\partial x_i} \tag{4.12}$$

and adopting Einstein's convention on repeated indices. Then we have

$$\langle (Tw)_\pm \rangle = \partial_i \langle p_i w_\pm + \alpha_i (w_2 \pm \nu_2 w_0) \rangle \mp \langle \vec{w} \cdot \Theta \vec{v} \rangle, \tag{4.13}$$

where we exploited the anti-symmetry of the operator Θ as an operator acting on functions of p (see definition (3.9)). This, in particular, implies that $\langle \Theta w \rangle = 0$ for all w. Let us now simply write g for $g[n]$. By putting $w = Tg$ in (4.13) we obtain a more explicit expression of the right-hand side of the quantum diffusive equations (4.9), which become

$$\partial_t n_\pm = \partial_i \partial_j \langle p_i p_j g_\pm + 2 p_i \alpha_j (g_2 \pm \nu_2 g_0) + \alpha_i \alpha_j (g_0 \pm \nu_2 g_2) \rangle$$
$$+ \partial_i \langle (p_i \pm \nu_2 \alpha_i) \Theta g_0 \pm p_i \vec{v} \cdot \Theta \vec{g} - 2\epsilon^{-1} \gamma \alpha_i g_1 \rangle$$
$$\mp \langle \Theta \vec{v} \cdot [p_i \partial_i \vec{g} + \Theta \vec{g} + \alpha_i \partial_i g_0 \vec{e}_2 - 2\epsilon^{-1} \vec{h} \times \vec{g}] \rangle, \tag{4.14}$$

with $g = g[n] = g[(n_+, n_-)]$. In order to complete the quantum diffusive model, a discussion is now required about the local equilibrium state represented by g. This will be done in the next section.

5 The Local Equilibrium Wigner Functions

In this section we describe the local equilibrium state $g = g_0 \sigma_0 + \vec{g} \cdot \vec{\sigma}$ as given by the quantum version of the minimum entropy principle. Then, g will be semiclassically expanded at first order in the semiclassical parameter ϵ.

5.1 Local Equilibrium State from Minimum Entropy Principle

Following Refs. [12, 13] we search the local-equilibrium state as the minimizer of a suitable quantum entropy-like functional $\mathcal{A}$, under the constraint that the moments under consideration are given. In our case, such moments are the two band-densities $n_\pm$ (see definition (3.7)). Assuming that the system is in thermal equilibrium with a bath at a given temperature T, the functional $\mathcal{A}$ will be the quantum Helmholtz free-energy functional

$$\mathcal{A}(S) = \text{Tr} \left\{ k_B T S \left(\log \frac{S}{N_0} - I \right) + H S \right\},$$

where S is the density operator describing the state of the system. Note that we are using the mathematician's convention for the sign of the entropy, opposed to the physicist's one. In scaled variables (see Sect. 3) $\mathcal{A}(S)$ reads as follows

$$\mathcal{A}(S) = \mathrm{Tr}\{S(\log S - I) + HS\}, \tag{5.1}$$

where, as usual, we adopt the same symbols for scaled and unscaled quantities.

Let us consider, therefore, the following constrained minimization problem.

Problem 5.1 *Let $n_+(x)$ and $n_-(x)$ be assigned functions. Find a density operator G such that $\mathcal{A}(G)$ is minimal among all density operators S satisfying $\langle w_\pm \rangle = n_\pm$, with $w = \mathrm{Op}_\epsilon^{-1}(S)$.*

Such operator will be our local-equilibrium density operator associated to n_+ and n_-. Adapting the proof given in Ref. [13] to the present (spinorial) case, we shall prove in the Appendix the following theorem.

Theorem 5.1 *A necessary condition for G to be a solution of the constrained minimization Problem 5.1 is that two functions $\mu_0(x)$ and $\mu_s(x)$ exist such that*

$$\begin{cases} G = \mathrm{e}^{-H_\mu}, \\ \langle g_\pm \rangle = n_\pm, & \text{with } g = \mathrm{Op}_\epsilon^{-1}(G), \end{cases} \tag{5.2}$$

where $H_\mu = \mathrm{Op}_\epsilon(h_\mu)$ is a modified $k \cdot p$ Hamiltonian with symbol

$$h_\mu(x, p) = [p^2/2 + V(x) + \mu_0(x)]\sigma_0 + [|\vec{h}(p)| + \mu_s(x)]\vec{v}(p) \cdot \vec{\sigma}. \tag{5.3}$$

Remark 5.1 Recalling (2.8) and (2.9), and putting

$$\mu_\pm(x) = V(x) + \mu_0(x) \pm \mu_s(x), \tag{5.4}$$

we can write

$$h_\mu(x, p) = [E_+(p) + \mu_+(x)]P_+(p) + [E_-(p) + \mu_-(x)]P_-(p), \tag{5.5}$$

where

$$E_\pm(p) = \frac{p^2}{2} \pm \sqrt{(\alpha \cdot p)^2 + \gamma^2} = \frac{p^2}{2} \pm |\vec{h}(p)| \tag{5.6}$$

are the scaled energy bands. From (5.5) we realize that H_μ provides each energy band with its own chemical potential. The two degrees of freedom represented by μ_+ and μ_- allows (in principle) the constraint equation $\langle g_\pm \rangle = n_\pm$ to be satisfied.

5.2 Associated Semigroup Equation

Several properties of G can be deduced from the associated semigroup equation for $G(\beta) = \mathrm{e}^{-\beta H_\mu}$, $\beta \geq 0$, that is

$$\begin{cases} \partial_\beta G(\beta) = -H_\mu G(\beta), & \beta > 0, \\ G(0) = I, \end{cases} \tag{5.7}$$

which, of course, yields G for $\beta = 1$. The corresponding equation for the Wigner matrix g is easily obtained by transforming system (5.7) with $\mathrm{Op}_\epsilon^{-1}$. This yields

$$\begin{cases} \partial_\beta g(\beta) = -h_\mu \#_\epsilon g(\beta), & \beta > 0, \\ g(0) = \sigma_0, \end{cases} \tag{5.8}$$

where $\#_\epsilon$ denotes the so-called Moyal (or "twisted") product between symbols [14, 39]

$$a \#_\epsilon b = \mathrm{Op}_\epsilon^{-1}[\mathrm{Op}_\epsilon(a)\,\mathrm{Op}_\epsilon(b)], \tag{5.9}$$

where a and b are 2×2 matrices, in the present case. The Moyal product has a semiclassical expansion

$$\#_\epsilon = \#^{(0)} + \epsilon \#^{(1)} + \epsilon^2 \#^{(2)} + \cdots, \tag{5.10}$$

where

$$a \#^{(k)} b = \frac{1}{(2i)^k} \sum_{|\alpha|+|\beta|=k} \frac{(-1)^{|\alpha|}}{\alpha!\beta!} (\partial_x^\alpha \partial_p^\beta a)(\partial_p^\alpha \partial_x^\beta b). \tag{5.11}$$

In particular, $\#^{(0)}$ is the usual matrix product,

$$a \#^{(0)} b = ab,$$

and $\#^{(1)}$ is the Poisson bracket between matrices

$$a \#^{(1)} b = \frac{i}{2} \sum_{k=1}^{3} \left(\frac{\partial a}{\partial x_k} \frac{\partial b}{\partial p_k} - \frac{\partial a}{\partial p_k} \frac{\partial b}{\partial x_k} \right).$$

As a first application of the semigroup equation (5.8), we show that our local equilibrium state satisfies condition (4.8) of Theorem 4.1.

Proposition 5.1 *A Wigner matrix $g(\beta)$ satisfying (5.8) is such that*

$$\langle (T g(\beta))_\pm \rangle = 0,$$

where T is given by (4.6). *In particular, the BGK equilibrium state $g[n^\tau]$ satisfies condition* (4.8) *for all $\tau \geq 0$.*

Proof Since $H_\mu G(\beta) = G(\beta) H_\mu$ and, therefore, $h_\mu \#_\epsilon g(\beta) = g(\beta) \#_\epsilon h_\mu$, then, using the fact that $\#^{(k)}$ is symmetric for even k and antisymmetric for odd k, the semigroup equation (5.8) can be expanded as

$$-\partial_\beta g(\beta) = \sum_{k \text{ even}} \epsilon^k [h_\mu \#^{(k)} g(\beta)]_+ + \sum_{k \text{ odd}} \epsilon^k [h_\mu \#^{(k)} g(\beta)]_-, \tag{5.12}$$

where $[ab]_+$ and $[ab]_-$ denote, respectively, the symmetric and antisymmetric part of the matrix product ab. The expressions in Pauli components are:

$$[ab]_+ = \begin{pmatrix} a_0 b_0 + \vec{a} \cdot \vec{b} \\ a_0 \vec{b} + \vec{a} b_0 \end{pmatrix}, \qquad [ab]_- = \begin{pmatrix} 0 \\ i\vec{a} \times \vec{b} \end{pmatrix}. \tag{5.13}$$

Now, let $\mathcal{C}$ denote the set of p-dependent 2×2 matrices a such that the Pauli components a_j are even functions of p for $j = 0, 1, 3$ and odd function of p for $j = 2$. Let us say, briefly, that $a \in \mathcal{C}$ has the parity structure

$$(\text{even, even, odd, even}).$$

It is immediate to see that the Hamiltonian symbol h_μ belongs to the parity class $\mathcal{C}$. Moreover, by using (5.11) and (5.13), it can be easily verified that, if $g \in \mathcal{C}$, then $[h_\mu \#^{(k)} g(\beta)]_+ \in \mathcal{C}$ for even k and $[h_\mu \#^{(k)} g(\beta)]_- \in \mathcal{C}$ for odd k. Since, clearly, $g(0) \in \mathcal{C}$, from the semigroup equation (5.8) (written in the form (5.12)) we immediately conclude that $g(\beta) \in \mathcal{C}$, for all $\beta \geq 0$. Now, it can be easily verified that, if $g(\beta) \in \mathcal{C}$, then $Tg(\beta)$ has the reverse parity structure (odd, odd, even, odd). Thus it turns out that $(Tg(\beta))_\pm$ are both odd functions of p and, consequently, $\langle (Tg(\beta))_\pm \rangle = 0$.

Since this result does not depend on the choice of the chemical potentials $\mu_\pm$ (or, equivalently, of the local densities $n_\pm$), then the BGK state $g[n^\tau]$, which just requires a particular choice of $\mu_\pm$, clearly satisfies (4.8). $\qquad\square$

5.3 Semiclassical Expansion of the Local Equilibrium Wigner Functions

As already remarked, the quantum diffusive equations (4.14) are formally closed if g can be expressed as a function of n_+ and n_- from the relation $\langle g_\pm \rangle = n_\pm$. The chemical potentials μ_+ and μ_- guarantee the necessary degrees of freedom. However, finding the explicit form of $\mu_\pm = \mu_\pm(n_+, n_-)$, and then of $g = g(n_+, n_-)$, is in general a very complicated task unless some approximations are performed. Since in standard applications the semiclassical parameter $\epsilon = \frac{\hbar}{p_0 x_0}$ is rather small (e.g. $\epsilon = 0.012$ for a system of typical size $x_0 = 10^{-7}$ m at a temperature $T = 300$ K), it is reasonable to assume $\epsilon \ll 1$ and investigate the semiclassical approximation of g and, consequently, of the quantum diffusive equations (4.14). A glance to (4.14) immediately suggests that also the ϵ-order approximation of g is needed to obtain the 0-order approximation of the diffusive equations.

Theorem 5.2 (Semiclassical expansion of the constrained entropy minimizer) *Assume that g satisfy the necessary conditions* (5.2). *Then*

$$g = g^{(0)} + \epsilon g^{(1)} + \mathcal{O}(\epsilon^2),$$

where $g^{(0)}$ is given (in Pauli components) by

$$g_0^{(0)} = \frac{\phi_+ + \phi_-}{2}, \qquad \vec{g}^{(0)} = \frac{\phi_+ - \phi_-}{2}\vec{v}, \tag{5.14}$$

with

$$\phi_\pm(x, p) = n_\pm(x)\,e^{-E_\pm(p)}/z_\pm, \qquad z_\pm := \int_{\mathbb{R}^3} e^{-E_\pm(p)}\,dp, \tag{5.15}$$

and $g^{(1)}$ is given by

$$g_0^{(1)} = 0, \qquad \vec{g}^{(1)} = \eta\vec{e}_1, \tag{5.16}$$

with $\vec{e}_1 = (1, 0, 0)$ and

$$\eta = \frac{\gamma \alpha_i}{4|\vec{h}|^2}\left[\partial_i(\phi_+ + \phi_-) + \frac{(\phi_+ - \phi_-)\partial_i \log(n_+ n_-)}{2|\vec{h}| - \log \frac{n_+ z_-}{z_+ n_-}}\right]. \tag{5.17}$$

Proof Let us assume for the moment that the chemical potentials do not depend on ϵ. As we have already seen, $g = g(\beta = 1)$, where $g(\beta)$ solves the semigroup problem (5.8). Let us, therefore, expand $g(\beta)$ in powers of ϵ:

$$g(\beta) = g^{(0)}(\beta) + \epsilon g^{(1)}(\beta) + \epsilon^2 g^{(2)}(\beta) + \cdots, \qquad (5.18)$$

Substituting (5.18) and (5.10) in (5.8) yields, at leading order,

$$\begin{cases} \partial_\beta g^{(0)}(\beta) = -h_\mu g^{(0)}(\beta), & \beta > 0, \\ g^{(0)}(0) = \sigma_0, \end{cases}$$

and, therefore,[1]

$$g^{(0)}(x, p; \beta) = e^{-\beta h_\mu(x,p)}.$$

After straightforward calculations we obtain the Pauli components of $g^{(0)} = g^{(0)}(\beta = 1)$:

$$g_0^{(0)} = \frac{\phi_+^\mu + \phi_-^\mu}{2}, \qquad \vec{g}^{(0)} = \frac{\phi_+^\mu - \phi_-^\mu}{2} \vec{v} \qquad (5.19)$$

where

$$\phi_\pm^\mu = \phi_\pm^\mu(x, p) = e^{-[E_\pm(p) + \mu_\pm(x)]}. \qquad (5.20)$$

As far as the first-order term is concerned, from (5.12) and (5.18) we obtain the equation for $g^{(1)}(\beta)$:

$$\begin{cases} \partial_\beta g^{(1)}(\beta) = -h_\mu g^{(1)}(\beta) - [h_\mu \#^{(1)} g^{(0)}(\beta)]_-, & \beta > 0, \\ g^{(1)}(0) = 0, \end{cases}$$

or

$$g^{(1)}(\beta) = -\int_0^\beta e^{-(\beta - \beta')h_\mu} [h_\mu \#^{(1)} g^{(0)}(\beta')]_- \, d\beta'.$$

After lengthy but straightforward calculations we obtain the Pauli components of $g^{(1)} = g^{(1)}(\beta = 1)$:

$$g_0^{(1)} = 0, \qquad \vec{g}^{(1)} = \eta^\mu \vec{e}_1, \qquad (5.21)$$

with $\vec{e}_1 = (1, 0, 0)$ and

$$\eta^\mu = -\frac{\gamma \alpha_i}{4|\vec{h}|^2} \left[\phi_+^\mu \partial_i \mu_+ + \phi_-^\mu \partial_i \mu_- + \frac{(\phi_+^\mu - \phi_-^\mu)\partial_i(\mu_+ + \mu_-)}{2|\vec{h}| + \mu_+ - \mu_-} \right], \qquad (5.22)$$

where $\phi_\pm^\mu$ are given by (5.20) and $\vec{h}$ by (3.16).

Now, $\mu_\pm$ depend on ϵ because the constraint equations in (5.2) contain ϵ. But, according to definition (4.2), we have $g_\pm^{(0)} = \phi_\pm^\mu$ and $g_\pm^{(1)} = 0$. Thus, the constraint equations imply

$$n_\pm = \langle g_\pm \rangle = \langle (g^{(0)} + \epsilon g^{(1)})_\pm \rangle + \mathcal{O}(\epsilon^2) = e^{-[E_\pm(p) + \mu_\pm(x)]} + \mathcal{O}(\epsilon^2),$$

---

[1] As expected, the semiclassical approximation of $\mathrm{Op}_\epsilon^{-1}(e^{-H_\mu})$ is simply given by the matrix exponential of the symbol Hamiltonian h_μ. Indeed, it can be proven that $\mathrm{Op}_\epsilon^{-1}[f(\mathrm{Op}_\epsilon(h))] \to f(h)$ for $\epsilon \to 0^+$, see Ref. [14].

which allows to invert at order 2 the relation between $\mu_\pm$ and $n_\pm$:

$$\mu_\pm = -\log\frac{n_\pm}{z_\pm} + \mathcal{O}(\epsilon^2), \tag{5.23}$$

with $z_\pm = \int_{\mathbb{R}^3} \mathrm{e}^{-E_\pm(p)} dp$. We see, therefore, that in (5.20) and (5.22) we can substitute $\mu_\pm$ with $-\log\frac{n_\pm}{z_\pm}$ by making an error of order ϵ^2. By performing such substitution in (5.20) we obtain (5.14)–(5.15). By performing the substitution in (5.22), we can first use the relation

$$\phi_\pm \partial_i \mu_\pm = -\partial_i \phi_\pm,$$

to get

$$\eta^\mu = \frac{\gamma \alpha_i}{4|\vec{h}|^2}\left[\partial_i(\phi_+ + \phi_-) - \frac{(\phi_+ - \phi_-)\partial_i(\mu_+ + \mu_-)}{2|\vec{h}| + \mu_+ - \mu_-}\right],$$

and then, by completing the substitution, we obtain (5.16)–(5.17). □

Remark 5.2 Intuitively enough, the leading-order semiclassical approximation of the local-equilibrium Wigner functions, $g^{(0)}$, is a couple of independent "Maxwellians", one for each band. The first-order correction $g^{(1)}$ is a peculiar feature of spinorial Hamiltonians, since it always vanishes in the scalar case.

6 Semiclassical Limits of the Diffusive Equation

As already remarked in the previous sections, the formal closure of the quantum diffusive equations (4.14) relies on the possibility of expressing the local-equilibrium Wigner functions g_k as functions of the moments n_+ and n_-. This (even in simpler non-spinorial situations) is in practice possible only in the semiclassical approximation $\epsilon \ll 1$. Thus, in this section we shall exploit the results of Sect. 5.3 in order to perform a leading-order semiclassical analysis of (4.14). This will be carried out for different scalings of the band parameters $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ and γ with respect to ϵ.

6.1 The Case $\alpha \sim 1$, $\gamma \sim 1$

First of all let us examine the case of a "strong influence" of the band parameters, which are therefore assumed to be of order 1 with respect to ϵ. The starting point are the quantum diffusive equations (4.14). There, the semiclassical parameter ϵ appears explicitly and is also hidden in $\Theta = \Theta_\epsilon[V]$ (see definition (3.9)) and in g (see previous section). As far as $\Theta_\epsilon[V]$ is concerned, its formal Taylor expansion in ϵ can be easily found and reads as follows:

$$\Theta_\epsilon[V] = \sum_{k=0}^{\infty} (-1)^{k+1}\left(\frac{\epsilon}{2}\right)^{2k} \sum_{|\alpha|=2k+1} \frac{1}{\alpha!} \nabla_x^\alpha V \nabla_p^\alpha. \tag{6.1}$$

Note that just the first term ($k = 0$) contributes to the leading order of (4.14), that is

$$\Theta_0[V] = -\nabla_x V \cdot \nabla_p, \tag{6.2}$$

which is nothing else than the force term in the classical Liouville equation. As far as g is concerned, we just need the $g^{(0)}$ and $g^{(1)}$ terms computed in the previous section and

given by (5.14)–(5.15) and (5.16)–(5.17), respectively. In particular, (5.14) implies $g_1^{(0)} = 0$ and $\vec{h} \times \vec{g}^{(0)} = 0$, and, therefore, no ϵ^{-1}-order terms will appear in our final equations. So, from (4.14) we see that what we have to compute is

$$
\begin{aligned}
\langle (TTg)_\pm^{(0)} \rangle =\ & \partial_i \partial_j \langle p_i p_j g_\pm^{(0)} + 2p_i \alpha_j (g_2^{(0)} \pm v_2 g_0^{(0)}) + \alpha_i \alpha_j (g_0^{(0)} \pm v_2 g_2^{(0)}) \rangle \\
& + \partial_i \langle (p_i \pm v_2 \alpha_i) \Theta_0 g_0^{(0)} \pm p_i \vec{v} \cdot \Theta_0 \vec{g}^{(0)} - 2\gamma \alpha_i g_1^{(1)} \rangle \\
& \mp \langle \Theta_0 \vec{v} \cdot [p_i \partial_i \vec{g}^{(0)} + \Theta_0 \vec{g}^{(0)} + \alpha_i \partial_i g_0^{(0)} \vec{e}_2 - 2\vec{h} \times \vec{g}^{(1)}] \rangle,
\end{aligned}
$$

where $\Theta_0 := \Theta_0[V]$ is given by (6.2). First of all, using (5.14) and $g_\pm^{(0)} = \phi_\pm$, we immediately obtain

$$
\begin{aligned}
\partial_i \partial_j \langle p_i p_j g_\pm^{(0)} &+ 2p_i \alpha_j (g_2^{(0)} \pm v_2 g_0^{(0)}) + \alpha_i \alpha_j (g_0^{(0)} \pm v_2 g_2^{(0)}) \rangle \\
&= \partial_i \partial_j \langle v_i^\pm v_j^\pm \phi_\pm \rangle + \partial_i \partial_j \langle c_{ij}^\pm (\phi_+ + \phi_-) \rangle,
\end{aligned} \tag{6.3}
$$

where

$$
v_i^\pm(p) := p_i \pm v_2 \alpha_i = p_i \pm \frac{\alpha_i \alpha \cdot p}{\sqrt{(\alpha \cdot p)^2 + \gamma^2}} = \frac{\partial E_\pm(p)}{\partial p_i} \tag{6.4}
$$

are the components of the electron semiclassical velocity in the two bands and, moreover, we have introduced the function

$$
c_{ij}^k = c_{ij}^k(p) := \frac{\gamma^2 \alpha_i \alpha_j}{2 |\vec{h}(p)|^k}. \tag{6.5}
$$

Next, let us compute the terms that depend on $g^{(0)}$ and are linear in Θ_0. By using the integration by parts and the following formula for the derivatives of $\vec{v}(p)$

$$
\frac{\partial}{\partial p_i} \vec{v}(p) = \frac{\gamma \alpha_i}{|\vec{h}(p)|^2} \vec{v}_\perp(p), \quad \vec{v}_\perp = (0, v_3, -v_2), \tag{6.6}
$$

we obtain

$$
\begin{aligned}
\partial_i \langle v_i^\pm \Theta_0 g_0^{(0)} &\pm p_i \vec{v} \cdot \Theta_0 \vec{g}^{(0)} \rangle \mp \langle \Theta_0 \vec{v} \cdot [p_i \partial_i \vec{g}^{(0)} + \alpha_i \partial_i g_0^{(0)} \vec{e}_2] \rangle \\
&= \partial_i [\partial_j V \langle \delta_{ij} \phi_\pm \pm 2 c_{ij}^3 (\phi_+ + \phi_-) \rangle] \mp \partial_i \partial_j V \langle c_{ij}^3 (\phi_+ + \phi_-) \rangle.
\end{aligned} \tag{6.7}
$$

As far as the term quadratic in Θ_0 is concerned, we obtain

$$
\langle \Theta_0 \vec{v} \cdot \Theta_0 \vec{g}^{(0)} \rangle = \partial_i V \partial_j V \langle c_{ij}^4 (\phi_+ - \phi_-) \rangle. \tag{6.8}
$$

Now, let us consider the contributions from $g^{(1)}$. Looking at (5.16)–(5.17), we can distinguish a linear part of $\vec{g}^{(1)}$,

$$
\vec{g}_{\text{lin}}^{(1)} = \frac{\gamma \alpha_i}{4 |\vec{h}|^2} \partial_i (\phi_+ + \phi_-) \vec{e}_1,
$$

and a nonlinear one,

$$
\vec{g}_{\text{nlin}}^{(1)} = -\frac{\gamma \alpha_i}{4 |\vec{h}|^2} \frac{(\phi_+ - \phi_-) \partial_i (\mu_+ + \mu_-)}{2 |\vec{h}| + \mu_+ - \mu_-} \vec{e}_1
$$

(in both cases $g_0^{(1)} = 0$).

As far as the linear part is concerned, we obtain

$$-\partial_i \langle 2\gamma\alpha_i\, g_{\text{lin},1}^{(1)}\rangle \pm \langle \Theta_0 \vec{v}\cdot 2\vec{h}\times\vec{g}_{\text{lin}}^{(1)}\rangle = -\partial_i\partial_j\langle c_{ij}^2(\phi_+ + \phi_-)\rangle$$
$$\mp \partial_i[\partial_j V\langle c_{ij}^3(\phi_+ + \phi_-)\rangle]$$
$$\pm \partial_i\partial_j V\langle c_{ij}^3(\phi_+ + \phi_-)\rangle. \qquad (6.9)$$

Putting together (6.3), (6.7), (6.8) and (6.9), we obtain the linear part of the semiclassical diffusive equation:

$$\langle (TTg)_\pm^{(0)}\rangle_{\text{lin}} = \partial_i\partial_j\langle v_i^\pm v_j^\pm \phi_\pm\rangle + \partial_i[\partial_j V\langle \delta_{ij}\phi_\pm \pm c_{ij}^3(\phi_+ + \phi_-)\rangle]$$
$$\mp \partial_i V\partial_j V\langle c_{ij}^4(\phi_+ - \phi_-)\rangle.$$

Remark 6.1 This expression is indeed linear in n_+ and n_-, because of the factorized structure of $\phi_\pm$ (see (5.15)). Using $\phi_+ + \phi_- = 2\phi_\pm \mp (\phi_+ - \phi_-)$, the previous equation can be rewritten as

$$\langle (TTg)_\pm^{(0)}\rangle_{\text{lin}} = \partial_i\partial_j\langle v_i^\pm v_j^\pm \phi_\pm\rangle + \partial_i[\partial_j V\langle (\delta_{ij}\pm 2c_{ij}^3)\phi_\pm\rangle]$$
$$- \partial_i[\partial_j V\langle c_{ij}^3(\phi_+ - \phi_-)\rangle]\mp \partial_i V\partial_j V\langle c_{ij}^4(\phi_+ - \phi_-)\rangle, \qquad (6.10)$$

putting in evidence a diagonal drift term in which the response of the band electron to the electric field is mediated by the tensor

$$\delta_{ij}\pm 2c_{ij}^3(p) = \delta_{ij}\pm \frac{\gamma^2\alpha_i\alpha_j}{|\vec{h}(p)|^3} = \frac{\partial^2 E_\pm(p)}{\partial p_i\partial p_j}, \qquad (6.11)$$

which is clearly related to the k·p effective-mass tensor [35]. Note that for certain values of the band parameters α and γ such effective-mass may be negative, making electrons in the lower band behave like holes.

Finally, let us consider the contribution from the nonlinear part of $g^{(1)}$ which, using (5.23), can be rewritten as follows:

$$\vec{g}_{\text{nlin}}^{(1)} = \frac{\gamma\alpha_i}{4|\vec{h}|^2}\frac{(\phi_+ - \phi_-)\partial_i\log(n_+ n_-)}{2|\vec{h}| - \log\frac{n_+ z_-}{z_+ n_-}}\vec{e}_1.$$

Using again (6.5) and (6.6), we quickly obtain

$$\langle (TTg)_\pm^{(0)}\rangle_{\text{nlin}} = -\partial_i\langle 2\gamma\alpha_i(g_{\text{nlin}}^{(1)})_1\rangle \pm \langle \Theta_0\vec{v}\cdot 2\vec{h}\times\vec{g}_{\text{nlin}}^{(1)}\rangle$$
$$= -\left\langle (c_{ij}^2\partial_i\pm c_{ij}^3\partial_i V)\frac{(\phi_+ - \phi_-)\partial_j\log(n_+ n_-)}{2|\vec{h}| - \log\frac{n_+ z_-}{z_+ n_-}}\right\rangle, \qquad (6.12)$$

which is, indeed, a nonlinear expression in n_+ and n_-. Putting together the linear and nonlinear parts, (6.10) and (6.12), and recalling the structure of $\phi_\pm$, see (5.15), we obtain the following result.

Theorem 6.1 (Formal semiclassical approximation for $\alpha \sim 1$, $\gamma \sim 1$) *Let us denote by $n^\epsilon_\pm$ the solution of the quantum diffusive equations* (4.14). *Then*

$$n^\epsilon_\pm = n_\pm + \mathcal{O}(\epsilon),$$

where $n_\pm$ satisfy the following system:

$$\partial_t n_\pm = \partial_i [D^\pm_{ij} \partial_j n_\pm + \partial_j V (\delta_{ij} \pm 2C^{3\pm}_{ij}) n_\pm]$$
$$- \partial_i [\partial_j V (C^{3+}_{ij} n_+ - C^{3-}_{ij} n_-)] \mp \partial_i V \partial_j V (C^{4+}_{ij} n_+ - C^{4-}_{ij} n_-)$$
$$- \int_{\mathbb{R}^3} (c^2_{ij} \partial_i \pm c^3_{ij} \partial_i V) \frac{(\phi_+ - \phi_-) \partial_j \log(n_+ n_-)}{2|\vec{h}| - \log \frac{n_+ z_-}{z_+ n_-}} \, dp, \qquad (6.13)$$

with

$$D^\pm_{ij} := \frac{1}{z_\pm} \int_{\mathbb{R}^3} v^\pm_i(p) v^\pm_j(p) \, e^{-E_\pm(p)} dp,$$
$$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (6.14)$$
$$C^{k\pm}_{ij} := \frac{1}{z_\pm} \int_{\mathbb{R}^3} c^k_{ij}(p) \, e^{-E_\pm(p)} dp.$$

We recall that $\phi_\pm$ are defined in (5.15), $v^\pm_i$ in (6.4) and c^k_{ij} in (6.5). Note that (6.13) is a nonlinear uniformly parabolic system because, as one can immediately see from (6.14), the 3×3 constant matrices D^+_{ij} and D^-_{ij} are definite positive. Note also that the parabolic system is not "weakly coupled" [29, 30], because of coupling terms involving derivatives of n_+ and n_-.

6.2 The Case $\alpha \sim \epsilon$, $\gamma \sim \epsilon$

We now consider the case in which both the band parameters, α and γ, have little influence on the dynamics at the macroscopic scale. We assume, therefore, that they are of order ϵ. In order to stress this fact, we make the substitutions

$$\alpha \to \epsilon\alpha, \qquad \gamma \to \epsilon\gamma, \qquad\qquad\qquad\qquad (6.15)$$

with $\alpha \sim 1$ and $\gamma \sim 1$ (of course, this amounts to redefine the change from unscaled to scaled quantities (3.14) as $\frac{mx_0\alpha}{\hbar} \to \alpha$, $\frac{mx_0\gamma}{p_0\hbar} \to \gamma$, and to assume $\frac{mx_0\alpha}{\hbar}$ and $\frac{mx_0\gamma}{p_0\hbar}$ to be of order 1). Note that the spinorial part of the Hamiltonian is rescaled as $\epsilon\vec{h}$ and, therefore, the energy bands are now

$$E^\epsilon_\pm(p) = \frac{p^2}{2} \pm \epsilon|\vec{h}(p)| = \frac{p^2}{2} \pm \epsilon\sqrt{(\alpha \cdot p)^2 + \gamma^2}.$$

Then, we should start again the whole procedure with the new scaled quantities: compute the new $g^{(0)}$ and $g^{(1)}$, as in Sect. 5, and compute the new right-hand side of the diffusive equation $\langle (TTg)^{(0)}_\pm \rangle$, as in Sect. 6.1. However, since the new problem is a regular perturbation of the previous one, an equivalent and much easier procedure is to start directly from the diffusive limit (6.13), insert the new factors ϵ where necessary, and just take the limit for $\epsilon \to 0$. To this aim, note that in such limit we have $E^\epsilon(p) \to p^2/2$ and then

$$\phi_\pm(x, p) \to n_\pm(x) e^{-p^2/2}/(2\pi)^{3/2}. \qquad\qquad\qquad (6.16)$$

Therefore, the leading order local-equilibrium distribution is now given by two identical Maxwellians in the two bands. Moreover, the semiclassical velocities $v^\pm$ (see (6.4)) both reduce to the "free" velocity p (we term it "velocity" because in unscaled variables it would be p/m). In particular, taking also into account (6.16), the diffusion coefficients $D_{ij}^\pm$ (see (6.14)) reduce to

$$D_{ij}^\pm \to \delta_{ij}.$$

Finally, since the coefficients $c_{ij}^k(p)$ (see (6.5)) scale as $\epsilon^{4-k} c_{ij}^k(p)$ we have that, in the limit $\epsilon \to 0$, only $k = 4$ survives. In particular, the integrated coefficient $C_{ij}^{4\pm}$ (see again (6.14) and use (6.16)) becomes

$$C_{ij}^{4\pm} \to \frac{\alpha_i \alpha_j \gamma^2}{2(2\pi)^{3/2}} \int_{\mathbb{R}^2} \frac{e^{-p^2/2}}{((\alpha \cdot p)^2 + \gamma^2)^2} \, dp := C_{ij} \tag{6.17}$$

(where, of course, α and γ are the crystal parameters in the new scaling). All this considered, making the substitutions (6.15) in (6.13) and passing to the limit $\epsilon \to 0$, we obtain the following result.

Theorem 6.2 (Formal semiclassical approximation for $\alpha \sim \epsilon$, $\gamma \sim \epsilon$) *Let us denote by $n_\pm^\epsilon$ the solution of the quantum diffusive equations* (4.14) *with α and γ substituted by $\epsilon\alpha$ and $\epsilon\gamma$. Then $n_\pm^\epsilon = n_\pm + \mathcal{O}(\epsilon)$, where $n_\pm$ satisfy the following system*:

$$\partial_t n_\pm = \partial_i(\partial_i n_\pm + \partial_i V n_\pm) \mp C_{ij} \partial_i V \partial_j V (n_+ - n_-), \tag{6.18}$$

and the coupling coefficients C_{ij} are given by (6.17).

Remark 6.2 Note that (6.18) are two standard drift-diffusion equations with a simple coupling term, proportional to the square of the force field, which acts as a relaxation mechanism for the band-polarity of the electron population (indeed, it is immediate to see from (6.17) that $\sum_{ij} C_{ij} \partial_i V \partial_j V \geq 0$).

6.3 The Case $\alpha \sim \epsilon$, $\gamma \sim 1$

We now assume that the coupling vector α is small, of order ϵ, while the band-gap parameter γ is of order 1. Thus, we now make the substitution

$$\alpha \to \epsilon\alpha, \tag{6.19}$$

with $\alpha \sim 1$ and $\gamma \sim 1$. Note that, in the limit $\epsilon \to 0$, we obtain

$$E_\pm^\epsilon(p) = \frac{p^2}{2} \pm \sqrt{\epsilon^2(\alpha \cdot p)^2 + \gamma^2} \quad \to \quad \frac{p^2}{2} \pm \gamma$$

and the energy bands reduce to two identical parabolic bands separated by a constant gap 2γ, while the Hamiltonian becomes diagonal. Hence, we expect that such limit describes two completely decoupled parabolic bands. Indeed, if we make the substitution (6.19) in (6.13) and pass to the limit, we easily see that

$$v_i^\pm \to p_i, \qquad D_{ij}^\pm \to \delta_{ij}, \qquad c_{ij}^k \to 0, \qquad C_{ij}^{k\pm} \to 0$$

and, therefore, we obtain the limit equations as follows.

Theorem 6.3 (Formal semiclassical approximation for $\alpha \sim \epsilon$, $\gamma \sim 1$) *Let us denote by $n_\pm^\epsilon$ the solution of the quantum diffusive equations* (4.14) *with α substituted by $\epsilon\alpha$. Then $n_\pm^\epsilon = n_\pm + \mathcal{O}(\epsilon)$, where $n_\pm$ satisfy the following system:*

$$\partial_t n_\pm = \partial_i (\partial_i n_\pm + \partial_i V n_\pm). \tag{6.20}$$

As expected, this is a trivial system of two decoupled diffusive equations for parabolic bands.

6.4 The Case $\alpha \sim 1$, $\gamma \sim \epsilon$

The last case we consider is when the coupling vector α is of order 1 and the band-gap parameter γ is of order ϵ. We therefore make the substitution

$$\gamma \to \epsilon\gamma, \tag{6.21}$$

with $\alpha \sim 1$ and $\gamma \sim 1$. Note that in this case the band-gap vanishes in the limit $\epsilon \to 0$ and the two bands become singular, with the appearance of a "Dirac plane" of equation $\alpha \cdot p = 0$ in the spectrum:

$$E_\pm^\epsilon(p) = \frac{p^2}{2} \pm \sqrt{(\alpha \cdot p)^2 + \epsilon^2 \gamma^2} \quad \rightarrow \quad E^0(p) = \frac{p^2}{2} \pm |\alpha \cdot p|.$$

Thus, unlike the preceding cases, this time we cannot expect a regular limit equation as $\epsilon \to 0$. Indeed, if we write explicitly the coupling coefficients $C_{ij}^{k,\pm}$ (see (6.14)) in the new scaling,

$$C_{ij}^{k\pm} = \frac{\epsilon^2 \gamma^2 \alpha_i \alpha_j}{z_\pm} \int_{\mathbb{R}^3} \frac{e^{-p^2/2 \mp \sqrt{(\alpha \cdot p)^2 + \epsilon^2 \gamma^2}}}{((\alpha \cdot p)^2 + \epsilon^2 \gamma^2)^{k/2}} \, dp,$$

we quickly see that

$$C_{ij}^{2\pm} \sim \epsilon, \qquad C_{ij}^{3\pm} \sim 1, \qquad C_{ij}^{4\pm} \sim \frac{1}{\epsilon},$$

showing that the coupling term $\partial_i V \partial_j V (C_{ij}^{4+} n_+ - C_{ij}^{4-} n_-)$ in the diffusive equations becomes singular. A more precise inspection, which starts again from the kinetic level and the quantum diffusive equation (4.14) (written in the new scaling), confirms that the term $\langle \Theta \vec{v} \cdot \Theta \vec{g} \rangle$ is of order $1/\epsilon$ and therefore singular. Hence, apparently, no semiclassical diffusive equation for the two band populations can be found in the scaling $\alpha \sim 1$, $\gamma \sim \epsilon$.

However, an alternative approach clarifies the situation. For $\gamma = 0$, let us change the definition of energy bands from the singular one, $E_\pm^0(p) = p^2/2 \pm |\alpha \cdot p|$, to the regular one,

$$E_\pm^*(p) = \frac{p^2}{2} \pm \alpha \cdot p. \tag{6.22}$$

Hence, the singular "upper" and "lower" bands are replaced by two regular bands that intersect along the plane $\alpha \cdot p = 0$. Note that, for such bands, the projection vector is given by $\vec{v}^* = \vec{e}_2 = (0, 1, 0)$. Using the new definition, it can be readily checked that the diffusive equations for

$$n_\pm^*(x, t) = \int_{\mathbb{R}^3} w_\pm^*(x, p, t) \, dp = \int_{\mathbb{R}^3} [w_0 \pm w_2](x, p, t) \, dp \tag{6.23}$$

in the limit $\epsilon \to 0$ read as follows:

$$\partial_t n_\pm^* = \partial_i [\partial_j \langle v_i^{*\pm} v_j^{*\pm} \phi_\pm^* \rangle + \partial_i V \langle \phi_\pm^* \rangle],$$

where

$$\phi_\pm^* = n_\pm^* e^{-E_\pm^*}/z_\pm^*, \qquad z_\pm^* = \int_{\mathbb{R}^3} e^{-E_\pm^*(p)} \, dp, \qquad v_i^{*\pm} = p_i \pm \alpha_i.$$

But, since

$$\langle v_i^{*\pm} v_j^{*\pm} e^{-E_\pm^*(p)}/z_\pm^* \rangle = \delta_{ij},$$

the above equations reduce to

$$\partial_t n_\pm^* = \partial_i (\partial_i n_\pm^* + \partial_i V n_\pm^*). \tag{6.24}$$

We can summarize the above discussion in the following Theorem.

Theorem 6.4 (Formal semiclassical approximation for $\alpha \sim 1$, $\gamma \sim \epsilon$) *Let us denote by $n_\pm^{*,\epsilon}$ the solution of the quantum diffusive equations* (4.9) *with γ substituted by $\epsilon\gamma$ and $(\cdot)_\pm$ substituted by $(\cdot)_\pm^*$, according to the new definition* (6.23). *Then*

$$n_\pm^{*,\epsilon} = n_\pm^* + \mathcal{O}(\epsilon),$$

where $n_\pm^*$ satisfy system (6.24).

Hence, the densities $n_\pm^*$ satisfy a decoupled system of drift-diffusion equations for parabolic bands. The reason becomes immediately clear by looking at the semiclassical dynamics in phase-space. Replacing γ by $\epsilon\gamma$ and letting $\epsilon \to 0$, the collisionless dynamics of the regular-band Wigner functions

$$w_\pm^* = w_0 \pm \vec{v}^* \cdot \vec{w} = w_0 \pm w_2$$

is readily derived from (3.15) and (6.2):

$$\partial_t w_\pm^* + (p \pm \alpha) \cdot \nabla_x w_\pm^* + F \cdot \nabla_p w_\pm^* = 0, \tag{6.25}$$

where $F = -\nabla_x V$ is the force field. The two families of particles are therefore decoupled and their diffusive regime is described by (6.24). On the other hand, the collisionless dynamics of the singular-band Wigner functions

$$w_\pm = w_0 \pm \vec{v} \cdot \vec{w} = w_0 \pm s w_2, \quad s = s(p) = \mathrm{sgn}(\alpha \cdot p),$$

is formally given by

$$\partial_t w_\pm + (p \pm s\alpha) \cdot \nabla_x w_\pm + F \cdot \nabla_p w_\pm = \pm 2\alpha \cdot F \delta(\alpha \cdot p) w_2,$$

which, using $w_2 = (w_+^* - w_-^*)/2$, can also be written

$$\partial_t w_\pm + (p \pm s\alpha) \cdot \nabla_x w_\pm + F \cdot \nabla_p w_\pm = \pm \alpha \cdot F \delta(\alpha \cdot p)(w_+^* - w_-^*). \tag{6.26}$$

The interpretation of these results is clear. The dynamics takes the simplest possible form when described in terms of $w_\pm^*$ but, if one wants to force the description in terms of $w_\pm$, a

coupling term concentrated on the Dirac plane appears which simply exchanges band labels in such a way to make (6.26) equivalent to (6.25). Note that such delta-like coupling term is the responsible for "squared delta" singularity in the squared transport operator TT which causes the failure of the semiclassical diffusive limit for $n_\pm$, as described above.

Remark 6.3 From the quantum-mechanical point of view, as already noticed in Sect. 2 (see Remark 2.2), we can observe that, if $\gamma = 0$, then energy eigenstates are simultaneously velocity eigenstates (and, of course, also eigenstates of the "pseudospin" σ_2). In particular, the states of energies $E_\pm^*(p)$ are also states, respectively, of velocity $p \pm \alpha$ (corresponding to pseudospin $\sigma_2 = \pm 1$). The same conclusion is not true for the bands $E_\pm(p)$ since, in that case, the pseudospin sign depends on the sign of $\alpha \cdot p$ (and, therefore, the pseudospin sign changes along each band when the Dirac plane is crossed). Thus, the decoupling of the bands $E_\pm^*$ can be interpreted in terms of pseudospin conservation across at the plane $\alpha \cdot p = 0$. A similar behavior has been predicted and observed at Dirac points in graphene [24, 38].

Appendix: Characterization of Local Equilibrium: Proofs

This Appendix is devoted to the proof of Theorem 5.1. First of all we note that the two constraints $\langle w_\pm \rangle = n_\pm$ are equivalent to the two constraints

$$\langle w_0 \rangle = n_0, \qquad \langle \vec{v} \cdot \vec{w} \rangle = n_s$$

because the moments (n_+, n_-) are clearly related to the moments (n_0, n_s) by $n_\pm = n_0 \pm n_s$. Thus, we can reformulate Problem 5.1 and Theorem 5.1 in the following equivalent form, where we recall that the quantum free-energy functional $\mathcal{A}(S)$ is

$$\mathcal{A}(S) = \text{Tr}\{S(\log S - I) + HS\}.$$

Problem A.1 *Let $n_0(x)$ and $n_s(x)$ be assigned functions. Find a density operator G such that $\mathcal{A}(G)$ is minimal among all density operators S satisfying $\langle w_0 \rangle = n_0$ and $\langle \vec{v} \cdot \vec{w} \rangle = n_s$, with $w = \text{Op}^{-1}(S)$.*

Theorem A.1 *A necessary condition for G to be a solution of the constrained minimization Problem A.1, is that two functions $\mu_0(x)$ and $\mu_s(x)$ exist such that*

$$\begin{cases} G = e^{-H_\mu}, \\ \langle g_0 \rangle = n_0, \; \langle \vec{v} \cdot \vec{g} \rangle = n_s, \quad \text{with } g = \text{Op}^{-1}(G), \end{cases} \tag{A.1}$$

where H_μ is given by the symbol (5.3).

Here and in the remainder of this section we have drop the unnecessary subscript ϵ from the Weyl quantization notation, so that $\text{Op} \equiv \text{Op}_\epsilon$.

By standard variational methods, the reformulated constrained minimization problem, Problem A.1, is equivalent to a saddle-point problem for the Lagrangian

$$\mathcal{L}(S, \mu) := \mathcal{A}(S) - \left[\mathcal{K}(S, \mu) - \int_{\mathbb{R}^3} (\mu_0 n_0 + \mu_s n_s)(x) \, dx \right], \tag{A.2}$$

where

$$\mathcal{K}(S, \mu) = \int_{\mathbb{R}^3} (\mu_0 \langle w_0 \rangle + \mu_s \langle \vec{v} \cdot \vec{w} \rangle)(x) \, dx, \quad w = \mathrm{Op}^{-1}(S),$$

and $\mu = (\mu_0, \mu_s)$, with $\mu_0 = \mu_0(x)$, $\mu_s = \mu_s(x)$ Lagrangian multipliers. Then, the constrained minimizer G must satisfy

$$\mathcal{A}(G) = \min_S \max_\mu \mathcal{L}(S, \mu) = \max_\mu \min_S \mathcal{L}(S, \mu).$$

Lemma 1 *Putting $f(S) = S(\log S - I)$, the Gâteaux derivative of $S \mapsto \mathrm{Tr}\{f(S)\}$ is given by*

$$\frac{\delta \, \mathrm{Tr}\{f(S)\}}{\delta S}(\delta S) = \mathrm{Tr}\{f'(S)\delta S\} = \mathrm{Tr}\{\log(S)\delta S\}.$$

Proof See [28] for a general result and [13] for an elementary proof restricted to $f \in C^1(0, +\infty)$, $f' > 0$, and $\mathrm{Tr}\{f(S)\}$ defined on density (i.e. trace-class, positive and self-adjoint) operators. □

Lemma 2 *A necessary condition for G_μ to be a solution of the unconstrained minimization problem*

$$\mathcal{L}(G_\mu, \mu) = \min_S \mathcal{L}(G_\mu, \mu) \tag{A.3}$$

is

$$G_\mu = \exp[-H - \mathrm{Op}(\mu_0 \sigma_0 + \mu_s \vec{v} \cdot \vec{\sigma})] = \exp(-H_\mu), \tag{A.4}$$

where $H_\mu = H + \mathrm{Op}(\mu_0 \sigma_0 + \mu_s \vec{v} \cdot \vec{\sigma})$, in accordance with the definition (5.3) of h_μ.

Note, therefore, that the chemical potentials introduced in Sect. 5 can now be interpreted as the Lagrangian multipliers associated to the constrained minimization problem.

Proof of Lemma 2 The Euler-Lagrange equation associated to the unconstrained minimization problem (A.3) is

$$\frac{\delta \mathcal{L}}{\delta S} = \frac{\delta \mathcal{A}}{\delta S} - \frac{\delta \mathcal{K}}{\delta S} = 0. \tag{A.5}$$

From Lemma 1 and the linearity of $\mathrm{Tr}\{HS\}$ we obtain

$$\frac{\delta \mathcal{A}}{\delta S}(\delta S) = \mathrm{Tr}\{\log(S)\delta S + H\delta S\}.$$

Recalling (3.5), the functional $\mathcal{K}$ can be written as follows:

$$\mathcal{K}(S, \mu) = \mathrm{Tr}\{\mathrm{Op}(\mu_0 \sigma_0 + \mu_s \vec{v} \cdot \vec{\sigma})S\}.$$

Thus, by linearity, we simply have

$$\frac{\delta \mathcal{K}}{\delta S}(\delta S) = \mathrm{Tr}\{\mathrm{Op}(\mu_0 \sigma_0 + \mu_s \vec{v} \cdot \vec{\sigma})\delta S\},$$

and the Euler-Lagrange equation (A.5) becomes

$$\text{Tr}\{\log(S)\delta S + H\delta S - \text{Op}(\mu_0\sigma_0 + \mu_s\vec{v}\cdot\vec{\sigma})\delta S\} = 0, \quad \forall \delta S. \tag{A.6}$$

The arbitrariness of the (self-adjoint, trace-class) variation δS implies that, if $S = G_\mu$ is a solution of (A.6), then G_μ must satisfy (A.4). □

Proof of Theorem A.1 From Lemma 2, the saddle-point problem (A.2) becomes the maximization problem

$$\mathcal{A}(G) = \max_\mu \min_S \mathcal{L}(S, \mu) = \max_\mu \mathcal{L}(G_\mu, \mu).$$

The Euler-Lagrange equation for such problem is

$$\frac{\delta\mathcal{L}}{\delta S}\bigg|_{(G_\mu,\mu)} \frac{\delta G_\mu}{\delta\mu} + \frac{\delta\mathcal{L}}{\delta\mu}\bigg|_{(G_\mu,\mu)} = 0,$$

which reduces to

$$\frac{\delta\mathcal{L}}{\delta\mu}\bigg|_{(G_\mu,\mu)} = 0$$

because (A.5) holds, being G_μ a minimizer. Now, by the linearity of $\mathcal{L}$ with respect to μ, we simply have

$$\frac{\delta\mathcal{L}}{\delta\mu}\bigg|_{(G_\mu,\mu)} = -\int_{\mathbb{R}^3} [\delta\mu_0(\langle g_0\rangle - n_0) + \delta\mu_s(\langle\vec{v}\cdot\vec{g}\rangle - n_s)](x)\,dx = 0$$

with $g = \text{Op}^{-1}(G_\mu)$. Since this equality must hold for any variation $(\delta\mu_0, \delta\mu_s)$, then we obtain the constraints

$$\langle g_0\rangle = n_0, \ \langle\vec{v}\cdot\vec{g}\rangle = n_s, \quad \text{with } g = \text{Op}^{-1}(G_\mu). \tag{A.7}$$

In conclusion, the constrained minimizer G must satisfy $G = G_\mu$, with G_μ given by (A.4) and satisfying (A.7). These conditions are exactly those of Theorem A.1. □

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