
BOLLETTINO UNIONE MATEMATICA ITALIANA

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*Bollettino dell'Unione Matematica Italiana, Serie 8, Vol. 8-B (2005),
n.1, p. 103–121.*

Unione Matematica Italiana

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Quantum Moment Equations for a Two-Band $k \cdot p$ Hamiltonian.

LUIGI BARLETTI (*)

Sunto. – *Vengono dedotte le equazioni per i momenti idrodinamici di un sistema quantistico descritto da un'Hamiltoniana $k \cdot p$ a due bande. Nel caso di stati puri si dimostra che le equazioni dei momenti di ordine 0 e di ordine 1 forniscono un sistema chiuso che costituisce l'analogo a due bande delle equazioni del fluido di Madelung.*

Summary. – *The hydrodynamic moment equations for a quantum system described by a two-band $k \cdot p$ Hamiltonian are derived. In the case of pure states, it is proved that the order-0 and order-1 moment equations yield a closed system which is the two-band analogue of Madelung's fluid equations.*

1. – Introduction.

Most mathematical models of quantum transport in semiconductor devices make use of the so-called *effective-mass approximation* [19, 20]. This amounts to substituting the complete Hamiltonian

$$(1.1) \quad H_{\text{complete}} = -\frac{\hbar^2}{2m}\Delta + V_{\mathcal{L}} + V,$$

where $V_{\mathcal{L}}$ is the periodic potential of the semiconductor crystal lattice and V accounts for other potentials, with the simplified effective-mass Hamiltonian

$$(1.2) \quad H_{\text{em}} = -\frac{\hbar^2}{2}\nabla^T M^{-1}\nabla + V.$$

Here, M is a suitable effective-mass tensor, rising up from a parabolic approxi-

(*) Comunicazione presentata a Milano in occasione del XVII Congresso U.M.I.

This research has been supported by the Italian MURST-COFIN2002 entitled *Problemi Matematici delle Teorie Cinetiche*, prot. 2002015553-003, and by the European RTN network *Hyperbolic and Kinetic Equations: Asymptotics, Numerics, Analysis*, ref. HPRN-CT-2002-00282.

mation of the conduction band $E_c(k)$ near a minimum point k^* [20]

$$(1.3) \quad M_{ij}^{-1} = \frac{\partial^2 E_c}{\partial k_i \partial k_j}(k^*).$$

Such approximation is good for electron wave numbers k close enough to k^* . Analogous considerations could be done for holes: they can be treated in the effective-mass approximation by using an effective-mass tensor obtained by a parabolic approximation of the valence band $E_v(k)$ near a maximum point.

It is important to stress the fact that the effective-mass approximation, by itself, does not supply any coupling mechanism between energy bands which, within this approximation, are always decoupled. This is the case of most bipolar electrons-holes models: for both kinds of carriers an effective-mass approximation is used and then a «generation-recombination» coupling term is heuristically inserted in the model [19].

However, in some cases a band-tunneling effect (the so-called Zener tunneling [12]) becomes the main feature of the semiconductor device. This is the case of recently developed devices, such as the Interband Resonant Tunneling Diode, where a conduction electron may become a valence electron after tunneling through a double barrier [21]. It is clear that a numerical simulation of such devices not accounting for band coupling would be unsatisfactory and, therefore, a mathematical model accounting at least for conduction-valence coupling must be developed.

The simplest Hamiltonian that allows to treat two coupled bands is the so-called $k \cdot p$ (« k dot p ») Hamiltonian [13, 17, 20]

$$(1.4) \quad H_{k \cdot p} = \begin{pmatrix} -\frac{\hbar^2}{2m} \Delta + V_1 & -\frac{\hbar^2}{m} K \cdot \nabla \\ \frac{\hbar^2}{m} K \cdot \nabla & -\frac{\hbar^2}{2m} \Delta + V_2 \end{pmatrix}.$$

Here, m is the electron mass and $K := \langle u_1 | \nabla | u_2 \rangle$, is the matrix element of the gradient operator between the (real) Bloch functions u_1 and u_2 , which is assumed to be constant. The functions V_1 and V_2 are the potentials of an electron in the conduction and in the valence band, respectively. In bulk crystals we can put $V_1 = V_2 + g$, where $g > 0$ is a constant band-gap. In other situations (such as in heterostructure devices) it may be convenient to let g be a function of the position. The interested reader may refer to Ref. [20] for more details.

The Hamiltonian (1.4) describes an electron that «sees» two energy bands available and, therefore, a Zener tunneling between the two bands is possible. It has to be remarked that also the $k \cdot p$ approximation holds for values of the electron wave numbers close to the extrema of the bands.

The aim of the present paper is to derive the equations of quantum hydrodynamic moments for the Hamiltonian (1.4). We recall that, for a «standard» quantum Hamiltonian

$$(1.5) \quad H = \frac{\hbar^2}{2m} \Delta + V$$

(which from now on will be referred to as a «one-band Hamiltonian»), quantum hydrodynamic (QHD) equations for pure quantum states were first deduced by Madelung in Ref. [18]. These are nowadays known as Madelung equations. More recently, a whole QHD theory has been developed in order to treat the much more difficult case of mixed quantum states, in which Madelung equations can still be written but are not closed any more (see Refs. [5, 10, 11]).

Generally speaking, there are at least two possible ways to derive QHD equations. One is deriving equations for densities and phases of WKB pure states, and then forming convex combinations to get equations for mixed states. The other is taking moments of quantum kinetic equations (viz. Wigner equations), in analogy to what is done in classical kinetic theory [15]. In such a «kinetic way to QHD» the following steps have therefore to be performed:

- I. writing a quantum kinetic equation,
- II. deriving the hierarchy of moment equations,
- III. truncating and closing the hierarchy.

For the single-band Hamiltonian (1.5), it turns out that, in the case of pure states, the system of order-0 and order-1 moment equations is closed and corresponds to Madelung equations.

In the present paper we wish to perform steps I and II for a quantum system governed by the $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian (1.4). We shall find a convenient way to write the hierarchy of moment equations and, moreover, we shall prove that for a pure state the system of order-0 and order-1 equations is closed, yielding «Madelung-like» two-band QHD equations.

2. – Moment equations for the free $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian.

We begin by considering the case of the «free» $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian

$$(2.1) \quad H_{\mathbf{k} \cdot \mathbf{p}}^0 := \begin{bmatrix} -\frac{\hbar^2}{2m} \Delta & -\frac{\hbar^2}{m} \mathbf{K} \cdot \nabla \\ \frac{\hbar^2}{m} \mathbf{K} \cdot \nabla & -\frac{\hbar^2}{2m} \Delta \end{bmatrix},$$

corresponding to (1.4) with $V_1 = V_2 = 0$. Note that we can write

$$(2.2) \quad H_{\mathbf{k}\cdot\mathbf{p}}^0 = \frac{P^2}{2m} - \frac{\hbar^2 K^2}{2m} I,$$

where I is the identity matrix and the momentum-like operator P is given by ⁽¹⁾

$$(2.3) \quad P := -i\hbar \begin{pmatrix} \nabla & K \\ -K & \nabla \end{pmatrix}.$$

Thus, the irrelevant, constant energy term $\frac{\hbar^2 K^2}{2m} I$ disappears from the Liouville equation

$$(2.4) \quad i\hbar \frac{\partial}{\partial t} S(t) = [H_{\mathbf{k}\cdot\mathbf{p}}^0, S(t)] = \frac{1}{2m} [P^2, S(t)],$$

describing the evolution of the time-dependent density operator $S(t)$ [3]. Note that the space of (pure) states for a two-band system described by Hamiltonian (1.4) or (2.1) is the same as for a spinning electron, i.e. $L^2(\mathbb{R}^d, \mathbb{C}^2)$ (with $d = 3$, but this is not crucial for our discussion). Thus $S(t)$, representing mixed states, is a self-adjoint 2×2 matrix of operators $S_{ij}(t)$, with $S_{ij}(t) = S_{ji}^*(t)$, where $i, j \in \{1, 2\}$ are the band indices. The corresponding density matrix $\varrho(t)$, i.e. the matrix of (formal) kernels of $S_{ij}(t)$, is given (using Dirac's notation) by

$$(2.5) \quad \varrho_{ij}(x, y, t) = \langle x, i | S(t) | y, j \rangle = \langle x | S_{ij}(t) | y \rangle.$$

The self-adjointness of $S(t)$ corresponds to the property

$$\varrho_{ij}(x, y, t) = \overline{\varrho_{ji}(y, x, t)}$$

of $\varrho(t)$. By using (2.4) and (2.5) we get the following equation for $\varrho(t)$:

$$(2.6) \quad i\hbar \frac{\partial}{\partial t} \varrho(t) = \frac{1}{2m} (P_x^2 - P_y^2) \varrho(t),$$

where we have found it convenient to introduce the shorthands

$$(2.7) \quad A_x := A \otimes I, \quad A_y := I \otimes A.$$

⁽¹⁾ The author is indebted to Naoufel Ben Abdallah for this remark.

This means that on a pure state $\varrho_{ij}(x, y) = \psi_i(x) \overline{\psi_j(y)}$ we put

$$(2.8) \quad \begin{aligned} (A_x \varrho)_{ij}(x, y) &= \sum_{k=1}^2 (A_{ik} \psi_k)(x) \overline{\psi_j(y)}, \\ (A_y \varrho)_{ij}(x, y) &= \psi_i(x) \sum_{k=1}^2 \overline{(A_{jk} \psi_k)(y)}; \end{aligned}$$

and then this formula is extended by linearity to mixed states, which are of the form $\varrho = \sum_{s=1}^{\infty} \lambda_s \varrho^s$, where $\lambda_s \geq 0$, $\sum_{s=1}^{\infty} \lambda_s = 1$ and each ϱ^s is a pure state, i.e. $\varrho_{ij}^s(x, y) := \psi_i^s(x) \overline{\psi_j^s(y)}$.

Since P_x and P_y commute, we can write $P_x^2 - P_y^2 = (P_x - P_y) \cdot (P_x + P_y)$ and the Liouville equation (2.6) is then recast into the following form:

$$(2.9) \quad \frac{\partial}{\partial t} \varrho(t) = \frac{1}{m} \frac{P_x - P_y}{i\hbar} \cdot \frac{P_x + P_y}{2} \varrho(t).$$

Let us now denote by $Wf = Wf(r, p)$, $(r, p) \in \mathbb{R}^d \times \mathbb{R}^d$ the Wigner transform of $f = f(x, y)$, $(x, y) \in \mathbb{R}^d \times \mathbb{R}^d$:

$$(2.10) \quad (Wf)(r, p) := \frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} f(r + \xi/2, r - \xi/2) e^{-i\xi \cdot p/\hbar} d\xi$$

(see Refs. [1, 7, 8, 16, 19]). We shall adopt the following notations:

1. if A is an operator acting in $L^2(\mathbb{R}^d, \mathbb{C})$, the operator obtained by similarity under the transformation W will be denoted by $\tilde{A}$, i.e.

$$(2.11) \quad \tilde{A} := WAW^{-1};$$

2. W is understood to act element by element on matrices, i.e.

$$W \begin{pmatrix} \varrho_{11} & \varrho_{12} \\ \varrho_{21} & \varrho_{22} \end{pmatrix} := \begin{pmatrix} W\varrho_{11} & W\varrho_{12} \\ W\varrho_{21} & W\varrho_{22} \end{pmatrix}.$$

We now want to write the equation governing the time-dependent Wigner matrix

$$(2.12) \quad w(t) := W\varrho(t),$$

where $\varrho(t)$ obeys (2.9). Note that, explicitly,

$$w(t) = \begin{pmatrix} w_{11}(r, p, t) & w_{21}(r, p, t) \\ w_{12}(r, p, t) & w_{22}(r, p, t) \end{pmatrix}$$

and $w_{ij}(r, p, t) = \overline{w_{ji}}(r, p, t)$. Thus, we have to transform eq. (2.9) by similarity, applying the transformation W , which leads to introducing the operators

$$(2.13) \quad \mathcal{O} := -W \left(\frac{P_x - P_y}{i\hbar} \right) W^{-1} = -\frac{\tilde{P}_x - \tilde{P}_y}{i\hbar}.$$

$$(2.14) \quad \mathcal{P} := W \left(\frac{P_x + P_y}{2} \right) W^{-1} = \frac{\tilde{P}_x + \tilde{P}_y}{2}.$$

By using the identities [1]

$$(2.15) \quad \tilde{\nabla}_x = \frac{\nabla_r}{2} + \frac{ip}{\hbar}, \quad \tilde{\nabla}_y = \frac{\nabla_r}{2} - \frac{ip}{\hbar},$$

and regarding w as the column-vector

$$w = \begin{pmatrix} w_{11} \\ w_{12} \\ w_{21} \\ w_{22} \end{pmatrix},$$

we can explicitly write the operators $\mathcal{O}$ and $\mathcal{P}$ as

$$(2.16) \quad \mathcal{O} = \nabla \mathbb{I} + K\mathbb{K}, \quad \mathcal{P} = p\mathbb{I} + \frac{i\hbar}{2}K\mathbb{J}$$

where $\mathbb{I}$ is the 4×4 identity matrix and

$$(2.17) \quad \mathbb{K} := \begin{pmatrix} 0 & 1 & 1 & 0 \\ -1 & 0 & 0 & 1 \\ -1 & 0 & 0 & 1 \\ 0 & -1 & -1 & 0 \end{pmatrix}, \quad \mathbb{J} := \begin{pmatrix} 0 & 1 & -1 & 0 \\ -1 & 0 & 0 & -1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & -1 & 0 \end{pmatrix}.$$

Using (2.9) and (2.11), we obtain the two-band Wigner equation [4, 6]

$$(2.18) \quad \frac{\partial}{\partial t} w(t) = -\frac{1}{m} \mathcal{O} \cdot \mathcal{P} w(t),$$

which is reminiscent of the usual Wigner equation for a free particle [1, 16, 19]

$$(2.19) \quad \frac{\partial}{\partial t} w(t) = -\frac{1}{m} \nabla_r \cdot p w(t).$$

Indeed, if we had used the single-band momentum operator $P = -i\hbar\nabla$, instead of the two-band momentum (2.3), we would have found $\mathcal{O} = \nabla$ and $\mathcal{P} = p$.

Let us now introduce the notation $\langle f \rangle = \langle f \rangle(r)$ for the «local average» of any phase-space quantity f :

$$(2.20) \quad \langle f \rangle(r) := \int_{\mathbb{R}^d} f(r, p) dp$$

(being understood that, if f is a matrix, or more generally a tensor, the average is taken element by element). We remark that, if $w = W\varrho$, then

$$(2.21) \quad \langle w \rangle(r) = \varrho(r, r) =: \langle \varrho \rangle(r)$$

which extends the bracket notation to ϱ . Note that we shall also write $\langle w \rangle(t)$ and $\langle \varrho \rangle(t)$ for $\langle w \rangle(r, t)$ and $\langle \varrho \rangle(r, t)$, omitting, as usual, all variables but time.

The advantage of having written the two-band Wigner equation in the form (2.18) is that this allows to take moment equations very easily. In fact, since the operator $\mathcal{O}$ does not involve the momentum variable p , then $\langle \mathcal{O} \cdot \rangle = \mathcal{O} \langle \cdot \rangle$. Therefore, from eq. (2.18) we get the order-0 moment equation

$$(2.22) \quad \frac{\partial}{\partial t} \langle w \rangle(t) + \frac{1}{m} \mathcal{O} \cdot \langle \mathcal{P} w \rangle(t) = 0.$$

Moreover, since $\mathcal{O}$ and $\mathcal{P}$ commute, we also have the order-1 moment equation

$$(2.23) \quad \frac{\partial}{\partial t} \langle \mathcal{P}^{\otimes n} w \rangle(t) + \frac{1}{m} \mathcal{O} \cdot \langle \mathcal{P} \otimes \mathcal{P} w \rangle(t) = 0.$$

More in general, the following order- n moment equation holds:

$$(2.24) \quad \frac{\partial}{\partial t} \langle \mathcal{P}^{\otimes n} w \rangle(t) + \frac{1}{m} \mathcal{O} \cdot \langle \mathcal{P}^{\otimes(n+1)} w \rangle(t) = 0,$$

where we put

$$(2.25) \quad \mathcal{P}^{\otimes n} := \overbrace{\mathcal{P} \otimes \mathcal{P} \otimes \dots \otimes \mathcal{P}}^{n \text{ times}}$$

Let us introduce the following notations:

$$(2.26) \quad n := \langle w \rangle, \quad J = \langle \mathcal{P} w \rangle \quad \text{and} \quad \text{Tr} \begin{bmatrix} a_{11} \\ a_{12} \\ a_{21} \\ a_{22} \end{bmatrix} := a_{11} + a_{22}.$$

Thus the order-0 equation (2.22) reads as follows

$$(2.27) \quad \frac{\partial n}{\partial t} + \frac{1}{m} \mathcal{O} \cdot J = 0$$

and, taking the trace, we obtain the conservation law

$$(2.28) \quad \frac{\partial \text{Tr} n}{\partial t} + \frac{1}{m} \nabla \cdot \text{Tr} \langle pw \rangle - \frac{2\hbar}{m} K \cdot \nabla \text{Im} n_{12} = 0.$$

Note that $\text{Tr} n = n_{11} + n_{22}$ is the total probability density, $\frac{1}{m} \text{Tr} \langle pw \rangle$ is the total probability current and $-\frac{2\hbar}{m} K \text{Im} n_{12}$ is an «interband current» [21].

3. – Temperature and Bohmian term.

We now focus our attention on the second-order moment $\langle \mathcal{P}^{\otimes 2} w \rangle = \langle \mathcal{P} \otimes \mathcal{P} w \rangle$. Recalling definitions (2.13) and (2.14), we can write

$$\begin{aligned} \mathcal{P}^{\otimes 2} &= \left(\frac{\tilde{P}_x + \tilde{P}_y}{2} \right)^{\otimes 2} = \frac{1}{4} (\tilde{P}_x^{\otimes 2} + 2 \tilde{P}_x \otimes \tilde{P}_y + \tilde{P}_y^{\otimes 2}) = \\ &= \frac{1}{4} (\tilde{P}_x - \tilde{P}_y)^{\otimes 2} + \tilde{P}_x \otimes \tilde{P}_y = -\frac{\hbar^2}{4} \mathcal{O}^{\otimes 2} + \tilde{P}_x \otimes \tilde{P}_y, \end{aligned}$$

where the (component-wise) commutativity between $\tilde{P}_x$ and $\tilde{P}_y$ was used. Note

also that $\tilde{P}_x$ and $\tilde{P}_y$ are now regarded as acting on column-vectors, rather than on matrices. Thus,

$$(3.1) \quad \langle \mathcal{P}^{\otimes 2} w \rangle = -\frac{\hbar^2}{4} \mathcal{O}^{\otimes 2} \langle w \rangle + \langle \tilde{P}_x \otimes \tilde{P}_y w \rangle.$$

Before going on, we introduce the following convention: every operation *between column-vectors* has to be understood component-wise. Thus, for example,

$$\begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix} := \begin{pmatrix} a_1 b_1 \\ a_2 b_2 \\ a_3 b_3 \\ a_4 b_4 \end{pmatrix}, \quad \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} / \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix} := \begin{pmatrix} a_1/b_1 \\ a_2/b_2 \\ a_3/b_3 \\ a_4/b_4 \end{pmatrix}$$

and, if a_i, b_i are d -vectors (such as the four components of $\langle \mathcal{P} w \rangle$),

$$\begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} \cdot \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix} := \begin{pmatrix} a_1 \cdot b_1 \\ a_2 \cdot b_2 \\ a_3 \cdot b_3 \\ a_4 \cdot b_4 \end{pmatrix} \quad \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} \otimes \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix} := \begin{pmatrix} a_1 \otimes b_1 \\ a_2 \otimes b_2 \\ a_3 \otimes b_3 \\ a_4 \otimes b_4 \end{pmatrix}$$

and so on. Bearing this in mind, we write

$$\begin{aligned} \langle \mathcal{P} w \rangle^{\otimes 2} &= \frac{1}{4} \langle (\tilde{P}_x + \tilde{P}_y) w \rangle^{\otimes 2} = \frac{1}{4} \left(\langle \tilde{P}_x w \rangle^{\otimes 2} + \langle \tilde{P}_y w \rangle^{\otimes 2} + 2 \langle \tilde{P}_x w \rangle \otimes \langle \tilde{P}_y w \rangle \right) = \\ &\quad \frac{1}{4} \langle (\tilde{P}_x - \tilde{P}_y) w \rangle^{\otimes 2} + \langle \tilde{P}_x w \rangle \otimes \langle \tilde{P}_y w \rangle \end{aligned}$$

and thus, using (2.13),

$$(3.2) \quad \langle \mathcal{P} w \rangle^{\otimes 2} = -\frac{\hbar^2}{4} \mathcal{O} \langle w \rangle^{\otimes 2} + \langle \tilde{P}_x w \rangle \otimes \langle \tilde{P}_y w \rangle.$$

Hence, using definitions (2.26), from (3.1) and (3.2) we get

$$(3.3) \quad \langle \mathcal{P} \otimes \mathcal{P} w \rangle = \frac{J \otimes J}{n} + Q(n) + nT,$$

where

$$(3.4) \quad Q(n) := -\frac{\hbar^2}{4} \left(\mathcal{O} \otimes \mathcal{O}n - \frac{(\mathcal{O}n) \otimes (\mathcal{O}n)}{n} \right)$$

and

$$(3.5) \quad nT := \langle \tilde{P}_x \otimes \tilde{P}_y w \rangle - \frac{\langle \tilde{P}_x w \rangle \otimes \langle \tilde{P}_y w \rangle}{n}.$$

Note that the first two terms of the right-hand side of eq. (3.3) depend only on n , J and their derivatives, while T depend on higher-order moments. In analogy with the single-band case [10, 11], $Q(n)$ is interpreted as a Bohmian «quantum pressure» and T as a «temperature».

PROPOSITION 3.1. – *Let $w = W_Q$ be the Wigner transform of the mixed state $\varrho = \sum_{s=1}^{\infty} \lambda_s \varrho^s$, where $\lambda_s \geq 0$, $\sum_{s=1}^{\infty} \lambda_s = 1$ and each ϱ^s is a pure state, i.e. $\varrho_{ij}^s(x, y) := \psi_i^s(x) \overline{\psi_j^s(y)}$. Thus*

$$(3.6) \quad T = \sum_{s=1}^{\infty} \frac{\lambda_s n^s}{n} \left(\frac{\langle P_x \varrho^s \rangle}{n^s} - \frac{\langle P_x \varrho \rangle}{n} \right) \otimes \left(\frac{\langle P_x \varrho^s \rangle}{n^s} - \frac{\langle P_x \varrho \rangle}{n} \right)^* =$$

$$= \sum_{s=1}^{\infty} \frac{\lambda_s n^s}{n} \left(\frac{\langle \tilde{P}_x w^s \rangle}{n^s} - \frac{\langle \tilde{P}_x w \rangle}{n} \right) \otimes \left(\frac{\langle \tilde{P}_x w^s \rangle}{n^s} - \frac{\langle \tilde{P}_x w \rangle}{n} \right)^*$$

where $w^s := W_{\varrho^s}$, $n^s := \langle \varrho^s \rangle = \langle w^s \rangle$ and $*$ denotes adjunction:

$$\begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix}^* := \begin{pmatrix} \bar{a}_1 \\ \bar{a}_3 \\ \bar{a}_2 \\ \bar{a}_4 \end{pmatrix}$$

PROOF. – Recalling (2.21) and (2.11) the equality between $\langle \tilde{P}_{x,y} w \rangle$ and $\langle P_{x,y} \varrho \rangle$ is clear (note also that we are regarding ϱ as a column vector). It is easier to work with density matrices rather than with Wigner functions. So, let us define q and q^s as follows:

$$(3.7) \quad q := \langle \tilde{P}_x w \rangle = \langle P_x \varrho \rangle = \sum_{s=1}^{\infty} \lambda_s \langle P_x \varrho^s \rangle =: \sum_{s=1}^{\infty} \lambda_s q^s.$$

Moreover, using $\langle P_x \varrho \rangle = \langle P_y \varrho \rangle^*$, it is easy to check that, for a pure state, we get

$$\langle P_x \otimes P_y \varrho^s \rangle = \frac{q^s \otimes (q^s)^*}{n^s}$$

and so, from definition (3.5),

$$\begin{aligned} T &= \frac{\langle P_x \otimes P_y \varrho \rangle}{n} - \frac{\langle P_x \varrho \rangle \otimes \langle P_y \varrho \rangle}{n^2} \\ &= \sum_{s=1}^{\infty} \lambda_s \frac{\langle P_x \otimes P_y \varrho^s \rangle}{n} - \frac{q \otimes q^*}{n^2} = \sum_{s=1}^{\infty} b^s \frac{q^s}{n^s} \otimes \frac{(q^s)^*}{n^s} - \frac{q \otimes q^*}{n^2} \end{aligned}$$

where

$$b^s := \frac{\lambda_s n^s}{n}.$$

Note that b_s is an r -dependent column-vector with non-negative first and fourth components and such that $\sum_{s=1}^{\infty} b^s$ has all the components equal to 1. Thus we get

$$T = \sum_{s=1}^{\infty} b^s \left(\frac{q^s}{n^s} - \frac{q}{n} \right) \otimes \left(\frac{q^s}{n^s} - \frac{q}{n} \right)^*,$$

i.e. eq. (3.6). ■

As an immediate consequence of Prop. 3.1, we have the following

COROLLARY 3.1. – *If w is the Wigner transform of a pure-state density matrix, then $T = 0$.*

It is worth remarking that in the single-band case, where $P = -i\hbar\nabla$, it turns out that

$$q = J + \frac{i\hbar}{2} \nabla n$$

and the decomposition (3.6) leads to a «current temperature»

$$T_c = \sum_{s=1}^{\infty} b^s \left(\frac{J^s}{n^s} - \frac{J}{n} \right) \otimes \left(\frac{J^s}{n^s} - \frac{J}{n} \right)^*,$$

plus an «osmotic temperature»

$$T_{os} = \frac{\hbar^2}{4} \sum_{s=1}^{\infty} b^s \left(\frac{\nabla n^s}{n^s} - \frac{\nabla n}{n} \right) \otimes \left(\frac{\nabla n^s}{n^s} - \frac{\nabla n}{n} \right)^*,$$

(see Refs. [10, 11]). Things are analogous here, in the two-band case, but far more complicated because of interband terms.

We can now write more explicitly the order-1 moment equation (2.23) in the following form:

$$(3.8) \quad \frac{\partial J}{\partial t} + \frac{1}{m} \mathcal{O} \cdot \left(\frac{J \otimes J}{n} + Q(n) + nT \right) = 0$$

For $T = 0$, we obtain from eqs. (2.27) and (3.8) a closed system of Madelung-like QHD equations for a free, two-band $k \cdot p$ Hamiltonian.

4. – Moments of the potential terms.

We now turn to the complete $k \cdot p$ Hamiltonian (1.4). Writing $H_{k \cdot p} = H_{k \cdot p}^0 + V$, where $H_{k \cdot p}^0$ is given by (2.1) and

$$(4.1) \quad V := \begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix},$$

the formalism introduced in Section 2 allows us to write the Wigner equation for the Hamiltonian $H_{k \cdot p}$ in the following form:

$$(4.2) \quad \frac{\partial}{\partial t} w(t) + \frac{1}{m} \mathcal{O} \cdot \mathcal{P} w(t) = \frac{1}{i\hbar} \mathfrak{V} w(t),$$

where we put

$$(4.3) \quad \mathfrak{V} := \tilde{V}_x - \tilde{V}_y$$

(see definitions (2.7) and (2.11)). Thus, the corresponding moment equations are

$$(4.4) \quad \frac{\partial}{\partial t} \langle \mathcal{P}^{\otimes n} w \rangle(t) + \frac{1}{m} \mathcal{Q} \cdot \langle \mathcal{P}^{\otimes(n+1)} w \rangle(t) = \frac{1}{i\hbar} \langle \mathcal{P}^{\otimes n} \nabla w \rangle(t), \quad n = 0, 1, 2, \dots$$

Using the column-vector representation for $\mathcal{Q}$ and w , we can write

$$V_x = V_1(x) \mathbb{I}_1^1 + V_2(x) \mathbb{I}_2^1, \quad V_y = V_1(y) \mathbb{I}_1^2 + V_2(y) \mathbb{I}_2^2,$$

where

$$(4.5) \quad \mathbb{I}_1^1 := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \mathbb{I}_2^1 := \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$\mathbb{I}_1^2 := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \mathbb{I}_2^2 := \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Thus, from standard results on Wigner transforms (see e.g. Ref. [1]) we have

$$(4.6) \quad \begin{aligned} \tilde{V}_x &= V_1 \left(r + \frac{i\hbar}{2} \nabla_p \right) \mathbb{I}_1^1 + V_2 \left(r + \frac{i\hbar}{2} \nabla_p \right) \mathbb{I}_2^1, \\ \tilde{V}_y &= V_1 \left(r - \frac{i\hbar}{2} \nabla_p \right) \mathbb{I}_1^2 + V_2 \left(r - \frac{i\hbar}{2} \nabla_p \right) \mathbb{I}_2^2, \end{aligned}$$

where the pseudo-differential operator $g(r, -i\hbar\nabla_p)$, acting on a phase-space function $f = f(r, p)$, is defined in the following way [8]:

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

The following proposition shows that, if the potentials V_1 and V_2 are regular enough, the local average $\langle \mathcal{P}^{\otimes n} \nabla w \rangle$ depends only on $\langle \mathcal{P}^{\otimes k} w \rangle$, with $k \leq n$. This

means that in the moment equations hierarchy (4.4) the potential terms do not cause «lack of closeness».

In what follows the standard multi-index notation will be used: a multi-index $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_d)$, is a d -tuple of non-negative integers and $|\alpha| := \alpha_1 + \alpha_2 + \dots + \alpha_d$, $\alpha! := \alpha_1! \alpha_2! \dots \alpha_d!$. Moreover $\alpha \leq \beta$ means $\alpha_i \leq \beta_i$ for $i = 1, 2, \dots, d$.

PROPOSITION 4.1. – Assume that V_1 and V_2 have derivatives of any order. Then, for any given $n = 0, 1, 2, \dots$, we can write (formally)

$$(4.7) \quad \langle \mathcal{P}^{\otimes n} \mathfrak{V} w \rangle = \sum_{|\alpha| \leq n} \sum_{j=1}^2 \left(\frac{-i\hbar}{2} \right)^{|\alpha|} \frac{\nabla^\alpha V_j}{\alpha!} F_{\alpha j}(\langle w \rangle, \langle \mathcal{P} w \rangle, \dots, \langle \mathcal{P}^{\otimes n'} w \rangle),$$

where the n -tensors $F_{\alpha j}$ are linear in each component of each argument and $n' \leq n - |\alpha|$.

PROOF. – Let us consider the expansion of the pseudo-differential operators appearing in (4.6) in a formal Taylor series with respect to $i\hbar \nabla_p$:

$$(4.8) \quad V_j \left(r \pm \frac{i\hbar}{2} \nabla_p \right) = \sum_{k=0}^{\infty} \sum_{|\alpha|=k} \left(\pm \frac{i\hbar}{2} \right)^k \frac{\nabla^\alpha V_j(r)}{\alpha!} \nabla_p^\alpha.$$

From eqs. (4.3), (4.6) and (4.8) we get

$$(4.9) \quad \mathfrak{V} = \sum_{k=0}^{\infty} \sum_{|\alpha|=k} \sum_{j=1}^2 \left(\frac{i\hbar}{2} \right)^k \frac{\nabla^\alpha V_j(r)}{\alpha!} \mathbb{H}_j^k \nabla_p^\alpha,$$

where $\mathbb{H}_j^k$ is defined in terms of the matrices $\mathbb{I}_j^i$ (see definition (4.5)) as follows

$$(4.10) \quad \mathbb{H}_j^k := \mathbb{I}_j^1 - (-1)^k \mathbb{I}_j^2.$$

for $j = 1, 2$ and $k = 0, 1, 2, \dots$. Thus, using (2.16) and (4.8), and putting

$$(4.11) \quad \tau := \frac{i\hbar}{2} K,$$

we can write

$$(4.12) \quad \langle \mathcal{P}^{\otimes n} \mathfrak{V} w \rangle = \sum_{k=0}^{\infty} \sum_{|\alpha|=k} \sum_{j=1}^2 \left(\frac{i\hbar}{2} \right)^k \frac{\nabla^\alpha V_j(r)}{\alpha!} \langle (p\mathbb{I} + \tau\mathbb{J})^{\otimes n} \mathbb{H}_j^k \nabla_p^\alpha w \rangle.$$

Now, if we consider a single component $(p\mathbb{I} + \tau\mathbb{J})^\beta$ of the tensor product

$(p\mathbb{I} + \tau\mathbb{J})^{\otimes n}$, (β is a multi-index with $|\beta| = n$), integration by parts yields

$$\langle (p\mathbb{I} + \tau\mathbb{J})^\beta \mathbb{H}_j^k \nabla_p^\alpha w \rangle = \begin{cases} (-1)^k \langle (p\mathbb{I} + \tau\mathbb{J})^{\beta-\alpha} \mathbb{H}_j^k w \rangle, & \text{if } \alpha \leq \beta \\ 0, & \text{if } \alpha \not\leq \beta \end{cases}$$

(recall that $|\alpha| = k$), from which we can see that the sum in eq. (4.12) is indeed extended only to $k \leq n$. We shall write, shortly,

$$\langle \mathcal{P}^{\otimes n} \mathbb{H}_j^k \nabla_p^\alpha w \rangle = (-1)^k \langle \mathcal{P}^{\otimes n-\alpha} \mathbb{H}_j^k w \rangle.$$

Let $\mathcal{P}' = (p\mathbb{I} + \tau\mathbb{J})^\gamma$, with $|\gamma| = n - k$, be any component of $\mathcal{P}^{\otimes n-\alpha}$. Then we can write

$$(p\mathbb{I} + \tau\mathbb{J})^\gamma = \sum_{\delta \leq \gamma} \binom{\gamma}{\delta} (p\mathbb{I})^\delta (\tau\mathbb{J})^{\gamma-\delta} = \sum_{\delta \leq \gamma} \binom{\gamma}{\delta} p^\delta \tau^{\gamma-\delta} \mathbb{J}^{|\gamma-\delta|},$$

and also

$$\begin{aligned} (p\mathbb{I} + \tau\mathbb{J})^\gamma \mathbb{H}_j^k &= \sum_{\delta \leq \gamma} \binom{\gamma}{\delta} \tau^{\gamma-\delta} \mathbb{J}^{|\gamma-\delta|} \mathbb{H}_j^k p^\delta = \sum_{\delta \leq \gamma} \binom{\gamma}{\delta} \tau^{\gamma-\delta} \mathbb{J}^{|\gamma-\delta|} \mathbb{H}_j^k (\mathcal{P} - \tau\mathbb{J})^\delta = \\ &\quad \sum_{\eta \leq \delta \leq \gamma} \binom{\gamma}{\delta} \binom{\delta}{\eta} \tau^{\gamma-\delta} \mathbb{J}^{|\gamma-\delta|} \mathbb{H}_j^k (-\tau\mathbb{J})^{\delta-\eta} \mathcal{P}^\eta \end{aligned}$$

where the commutativity between $\mathcal{P}$ and $\tau\mathbb{J}$ has been used. This shows that each component of $\langle \mathcal{P}^{\otimes n-\alpha} \mathbb{H}_j^k w \rangle$ is a linear combination of terms $\langle \mathcal{P}^\eta w \rangle$, with $|\eta| \leq n - k$.

In conclusion, we have written

$$\langle \mathcal{P}^{\otimes n} \nabla w \rangle = \sum_{k=0}^n \sum_{|\alpha|=k} \sum_{j=1}^2 \left(\frac{-i\hbar}{2} \right)^k \frac{\nabla^\alpha V_j(r)}{\alpha!} \langle \mathcal{P}^{\otimes n-\alpha} \mathbb{H}_j^k w \rangle,$$

and shown that $\langle \mathcal{P}^{\otimes n-\alpha} \mathbb{H}_j^k w \rangle$ is a linear combination of components of $\langle \mathcal{P}^{\otimes n'} w \rangle$, with $n' \leq n - |\alpha|$, which proves eq. (4.7). ■

5. – Two-band Madelung equations.

Propositions 3.1 and 4.1 imply that the $n = 0$ and $n = 1$ moment equations (4.4) for a pure state (i.e. with $T = 0$) are closed and yield a two-band analogue of QHD Madelung equations. In order to write such equations

we shall express in a more explicit form the moments of the potential term, (4.7), up to $n = 1$.

For $n = 0$, recalling definitions (4.5) and (4.10)

$$(5.1) \quad \langle \nabla w \rangle = V_1 \mathbb{H}_1^0 \langle w \rangle + V_2 \mathbb{H}_2^0 \langle w \rangle = g \mathbb{G} \langle w \rangle,$$

where

$$(5.2) \quad \mathbb{G} := \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

and $g := V_1 - V_2$ is the band-gap.

For $n = 1$ and $k = 0$, recalling (2.16) and (4.11), we have a contribution

$$(5.3) \quad \sum_{j=1}^2 \langle V_j \mathcal{P} \mathbb{H}_j^0 w \rangle = g \langle \mathcal{P} \mathbb{G} w \rangle = g \langle \mathbb{G} \mathcal{P} w + [\mathcal{P}, \mathbb{G}] w \rangle =$$

$$g \mathbb{G} \langle \mathcal{P} w \rangle + g \tau[\mathbb{J}, \mathbb{G}] \langle w \rangle = g \mathbb{G} \langle \mathcal{P} w \rangle + \frac{i\hbar g}{2} K[\mathbb{J}, \mathbb{G}] \langle w \rangle,$$

where

$$[\mathbb{J}, \mathbb{G}] = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}.$$

Finally, the contribution of $n = 1$ and $k = 1$ is

$$(5.4) \quad \sum_{|\alpha|=1} \sum_{j=1}^2 \frac{-i\hbar}{2} \nabla^\alpha V_j(r) \cdot \langle \nabla_p^\alpha \mathcal{P} \mathbb{H}_j^1 w \rangle = \sum_{j=1}^2 \frac{-i\hbar}{2} \nabla V_j(r) \mathbb{H}_j^1 \langle w \rangle = -i\hbar \nabla \mathbb{E} \langle w \rangle,$$

where

$$\mathbb{E} := \begin{pmatrix} V_1 & 0 & 0 & 0 \\ 0 & \frac{V_1 + V_2}{2} & 0 & 0 \\ 0 & 0 & \frac{V_1 + V_2}{2} & 0 \\ 0 & 0 & 0 & V_2 \end{pmatrix}.$$

Using eqs. (3.3), (5.1), (5.3), (5.4) and recalling definitions (2.26), we can write the moment equations (4.4) for $n = 0$ and $n = 1$ in the following form:

$$(5.5a) \quad \frac{\partial}{\partial t} n + \frac{1}{m} \mathcal{O} \cdot J = \frac{g}{i\hbar} G n$$

$$(5.5b) \quad \frac{\partial}{\partial t} J + \frac{1}{m} \mathcal{O} \cdot \left(\frac{J \otimes J}{n} + Q(n) + nT \right) = \frac{g}{i\hbar} G J + \frac{g}{2} K[J, G] n - \nabla E n ,$$

where $Q(n)$ is given by (3.4) and T is given by (3.5). By putting $T = 0$ in eqs. (5.5) we obtain a closed Madelung-like system, governing the evolution of a pure state.

In conclusion, we have written the hierarchy of moment equations for the two-band $k \cdot p$ Hamiltonian (1.4) (eqs. (4.4)) and shown that, for regular potentials, the coupling with higher-order moments is only due to the flow terms $\mathcal{O} \cdot \langle \mathcal{P}^{\otimes(n+1)} w \rangle$ (Prop. 4.1). Moreover, the first two moment equations with zero temperature ($T = 0$) are decoupled from the rest of the hierarchy and so they yield a closed, Madelung-like system (eqs. (5.5)).

There are many problems left open here. Besides purely mathematical problems, such as the well-posedness of system (5.5) with $T = 0$ or its equivalence with Schrödinger equation (which are already very difficult questions in the single-band case [11]), there is the big point of finding closures, even at a formal level, of the moment equations in the mixed-state case ($T \neq 0$). It seems that, in principle, there are at least two possibilities to achieve this. One, in analogy with the method followed by Gardner in the single-band case [9], is using a «local version» of the Wigner distribution at thermal equilibrium, semi-classically approximated at order $\hbar^2$ (such semi-classical approximation has been calculated for the Hamiltonian (1.4) in Ref. [2]). The other is following the approach of Degond and Ringhofer [5], which is the quantum analogue of Levermore's moment closure theory [15].

We end by a last remark: the method introduced in Sec. 2 for deriving moment equations may be adapted to a more general class of quantum systems, such as particles with spin or multi-band $k \cdot p$ Hamiltonians. As an example, let us apply our method to the Hamiltonian of the electron in an electromagnetic field

$$H = \frac{1}{2m} \left(i\hbar \nabla + \frac{e}{c} A \right)^2 + e\phi .$$

In this case we take $P := -i\hbar\nabla - \frac{e}{c}A$ and it is not an hard task showing that

$$\langle \mathcal{O}w \rangle = \nabla_r \langle w \rangle \quad \text{and} \quad \langle \mathcal{P}w \rangle = \langle pw \rangle - \frac{e}{c}A \langle w \rangle.$$

Note, in particular, that $\langle \mathcal{P}w \rangle$ is the so-called Pauli current [14]. However, the problem of finding conditions under which our method can be generalized to other Hamiltonians deserves a deeper investigation and is deferred to a future work.

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Pervenuta in Redazione
l'1 dicembre 2001