

Quantum Moment Equations for a One-Band and a Two-Band kp Pauli-type Hamiltonian

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Abstract

The hydrodynamic moment equations for a quantum system described by a One-Band Pauli type Hamiltonian and a Two-Band kp Pauli type Hamiltonian are derived.

Keywords: quantum moment equations, Pauli-type Hamiltonian

1. Introduction

In (Wigner, 1932) E. Wigner introduced the quasi-distribution

$$w(r, p) = \frac{1}{h^d} \int_{\mathbb{R}^d} \rho\left(r + \frac{\xi}{2}, r - \frac{\xi}{2}\right) e^{-i\frac{p\xi}{\hbar}} d\xi \quad (1)$$

for a quantum system with d degrees of freedom in the mixed state described by the density matrix

$$\rho(x, y) = \langle x|S|y\rangle \quad (2)$$

corresponding to the statistical operator S . As usual h denotes the Planck constant and $\hbar = \frac{h}{2\pi}$.

In (Barletti, 2005), L. Barletti, studied the Quantum Moment Equations for the Two-Band Kp Hamiltonian of this type

$$H_{Kp} = \begin{pmatrix} -\frac{\hbar^2}{2m}\Delta + V_1 & -\frac{\hbar^2}{m}K\nabla \\ \frac{\hbar^2}{m}K\nabla & -\frac{\hbar^2}{2m}\Delta + V_2 \end{pmatrix} \quad (3)$$

where m is the electron mass, $K = \langle u_1|\nabla|u_2\rangle$ is the matrix element of the gradient operator between the real Bloch function u_1 and u_2 which is assumed to be constant and the functions V_1, V_2 are the potentials of the electron in the conduction and in the valence band respectively. The Hamiltonian (3) describes an electron that "sees" two energy bands available and a Zener tunneling between the two-band is possible. This is the case of Interband Resonant Tunneling Diode where a conduction electron may become a valence electron after tunneling through a double barrier (Borgioli, Frosali, Zweifel, 2003). If we work with the (3) Hamiltonian we don't consider the electron as a $1/2$ spin particle.

We will consider the following One-Band Pauli Hamiltonian

$$H_P = \left[\frac{1}{2m} \left(\frac{\hbar}{i}\nabla - \frac{e}{c}A \right)^2 + e\phi \right] \sigma_0 - \frac{e\hbar}{2mc} B^i \sigma_i \quad (4)$$

where

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

with

$$A = (A^1(x), A^2(x), A^3(x)), B = (B^1(x), B^2(x), B^3(x))$$

and $B = \text{curl}(A)$; we will derive the equations of quantum hydrodynamic moments for this type of Hamiltonian. Moreover we study the Two-band case, too. These types of Hamiltonian operators consider the electron as a 1/2 spin particle.

We will derive the equations of quantum hydrodynamic moments for this type of Hamiltonians and we prove for a pure state the system of order-0 and order-1 equations is closed.

2. Moment Equations for the Pauli Hamiltonian

We start to consider the Pauli Hamiltonian

$$H_P = \left[\frac{1}{2m} \left(\frac{\hbar}{i} \nabla - \frac{e}{c} A \right)^2 + e\phi \right] \sigma_0 - \frac{e\hbar}{2mc} B^i \sigma_i$$

let us take

$$H_P = H^i \sigma_i = \sum_{i=0}^4 H^i \sigma_i \tag{5}$$

with $H^0 = \left[\frac{1}{2m} \left(\frac{\hbar}{i} \nabla - \frac{e}{c} A \right)^2 + e\phi \right]$ and $H^i = -\frac{e\hbar}{2mc} B^i$, for $i = 1, 2, 3$; then for the density matrix we get

$$\begin{aligned} i\hbar \partial_t \varrho &= H_x^i \sigma_i \varrho - H_y^i \varrho \sigma_i \\ &= \frac{1}{2} H_x^i \sigma_i \varrho + \frac{1}{2} H_x^i \sigma_i \varrho \\ &\quad + \frac{1}{2} H_y^i \sigma_i \varrho - \frac{1}{2} H_y^i \varrho \sigma_i - \\ &\quad - \frac{1}{2} H_y^i \varrho \sigma_i - \frac{1}{2} H_x^i \varrho \sigma_i + \\ &\quad + \frac{1}{2} H_x^i \varrho \sigma_i - \frac{1}{2} H_x^i \varrho \sigma_i \\ &= \frac{1}{2} (H_x^i + H_y^i) \sigma_i \varrho + \\ &\quad + \frac{1}{2} (H_x^i - H_y^i) \sigma_i \varrho - \\ &\quad - \frac{1}{2} (H_x^i + H_y^i) \varrho \sigma_i + \\ &\quad + \frac{1}{2} (H_x^i - H_y^i) \varrho \sigma_i \\ &= \frac{1}{2} (H_x^i + H_y^i) [\sigma_i, \varrho]_- + \\ &\quad + \frac{1}{2} (H_x^i - H_y^i) [\sigma_i, \varrho]_+ \end{aligned} \tag{6}$$

where $[a, b]_{\pm} = ab \pm ba$.

From (6) we obtain

$$\begin{aligned} i\hbar \partial_t \varrho &= \frac{1}{2m} \left[\left(\frac{\hbar}{i} \nabla_x - \frac{e}{c} A(x) \right)^2 - \left(\frac{\hbar}{i} \nabla_y - \frac{e}{c} A(y) \right)^2 \right] \varrho + \\ &\quad + e(\phi(x) - \phi(y)) \varrho - \\ &\quad - \frac{e\hbar}{4mc} (B^i(x) - B^i(y)) [\sigma_i, \varrho]_+ - \\ &\quad - \frac{e\hbar}{4mc} (B^i(x) + B^i(y)) [\sigma_i, \varrho]_- \end{aligned} \tag{7}$$

with $\varrho = \begin{pmatrix} \varrho_{1,1} & \varrho_{1,2} \\ \varrho_{2,1} & \varrho_{2,2} \end{pmatrix}$ and $\varrho_{1,2}(x, y; t) = \varrho_{2,1}^*(y, x; t)$.

Let us take $P = \frac{\hbar}{i} \nabla - \frac{e}{c} A$, then by (7) we get

$$\begin{aligned} i\hbar \partial_t \varrho &= \frac{1}{2m} (P_x^2 - P_y^2) \varrho + e(\phi(x) - \phi(y)) \varrho - \\ &\quad - \frac{e\hbar}{4mc} \left[(B^i(x) - B^i(y)) [\sigma_i, \varrho]_+ + (B^i(x) + B^i(y)) [\sigma_i, \varrho]_- \right] \end{aligned} \tag{8}$$

and

$$\begin{aligned} \partial_t \varrho &= \frac{1}{m} \left[\left(\frac{P_x - P_y}{2} \right) \left(\frac{P_x + P_y}{i\hbar} \right) \right] \varrho - \frac{ei}{\hbar} (\phi(x) - \phi(y)) \varrho + \\ &\quad + \frac{ei}{4mc} \left[(B^i(x) - B^i(y)) [\sigma_i, \varrho]_+ + (B^i(x) + B^i(y)) [\sigma_i, \varrho]_- \right]. \end{aligned} \tag{9}$$

By Wigner transform we have

$$\begin{aligned} \partial_t w &= \frac{1}{m} \widetilde{P}_r \widetilde{P}_p w - \frac{ei}{\hbar} \Theta_- (\phi) w + \\ &\quad + \frac{ei}{4mc} \left[\Theta_- (B^i) [\sigma_i, w]_+ + \Theta_+ (B^i) [\sigma_i, w]_- \right] \end{aligned} \tag{10}$$

where $w = \mathcal{W}_Q$ and

$$\begin{aligned} \widetilde{\mathcal{P}}_r &= \mathcal{W} \left(\frac{P_x + P_y}{i\hbar} \right) \mathcal{W}^{-1} \\ &= \mathcal{W} \left(\frac{\hbar}{i} \frac{\nabla_x + \nabla_y}{i\hbar} \right) \mathcal{W}^{-1} + \\ &\quad + \frac{e}{i\hbar c} \mathcal{W} (A(x) + A(y)) \mathcal{W}^{-1} \\ &= P_r + \frac{e}{i\hbar c} \Theta_+(A) \\ \widetilde{\mathcal{P}}_p &= \mathcal{W} \left(\frac{P_x - P_y}{2} \right) \mathcal{W}^{-1} \\ &= \frac{\hbar}{i} \mathcal{W} \left(\frac{\nabla_x - \nabla_y}{2} \right) \mathcal{W}^{-1} + \\ &\quad + \frac{e}{2c} \mathcal{W} (A(x) - A(y)) \mathcal{W}^{-1} \\ &= P_p + \frac{e}{2c} \Theta_-(A) \end{aligned}$$

with

$$\begin{aligned} \widetilde{\nabla}_x &= \mathcal{W} (\nabla_x) \mathcal{W}^{-1} \\ &= \frac{\nabla_x}{2} + \frac{i}{\hbar} p \\ \widetilde{\nabla}_y &= \mathcal{W} (\nabla_y) \mathcal{W}^{-1} \\ &= \frac{\nabla_y}{2} - \frac{i}{\hbar} p \\ \widetilde{P}_r &= \frac{\hbar}{i} \mathcal{W} \left(\frac{\nabla_x + \nabla_y}{i\hbar} \right) \mathcal{W}^{-1} \\ &= \frac{\hbar}{i} \frac{\widetilde{\nabla}_x + \widetilde{\nabla}_y}{i\hbar} = -\nabla_r \\ \widetilde{P}_p &= \frac{\hbar}{i} \mathcal{W} \left(\frac{\nabla_x - \nabla_y}{2} \right) \mathcal{W}^{-1} \\ &= \frac{\hbar}{i} \frac{\widetilde{\nabla}_x - \widetilde{\nabla}_y}{2} = p \end{aligned}$$

and

$$\begin{aligned} \Theta_-(\phi)(\cdot) &= (2\pi)^{-3} \int_{\mathbb{R}^6} \left[\phi \left(r + \frac{\hbar}{2} \xi \right) - \phi \left(r - \frac{\hbar}{2} \xi \right) \right] (\cdot) e^{-i(p-p_1)\xi} dp_1 d\xi \\ \Theta_{\pm}(A^j)(\cdot) &= (2\pi)^{-3} \int_{\mathbb{R}^6} \left[A^j \left(r + \frac{\hbar}{2} \xi \right) \pm A^j \left(r - \frac{\hbar}{2} \xi \right) \right] (\cdot) e^{-i(p-p_1)\xi} dp_1 d\xi \\ \Theta_{\pm}(B^j)(\cdot) &= (2\pi)^{-3} \int_{\mathbb{R}^6} \left[B^j \left(r + \frac{\hbar}{2} \xi \right) \pm B^j \left(r - \frac{\hbar}{2} \xi \right) \right] (\cdot) e^{-i(p-p_1)\xi} dp_1 d\xi \end{aligned} \tag{11}$$

for $j = 1, 2, 3$; moreover

$$\begin{aligned} \widetilde{P}_x &= \mathcal{W} \left(\frac{\hbar}{i} \nabla_x - \frac{e}{c} A(x) \right) \mathcal{W}^{-1} \\ &= \frac{\hbar}{i} \widetilde{\nabla}_x - \frac{e}{c} \widetilde{A}_x \\ &= \frac{\hbar}{i} \frac{\nabla_x}{2} + p - \frac{e}{c} \widetilde{A}_x; \\ \widetilde{P}_y &= \frac{\hbar}{i} \mathcal{W} \left(\frac{\hbar}{i} \nabla_y - \frac{e}{c} A(y) \right) \mathcal{W}^{-1} \\ &= \frac{\hbar}{i} \widetilde{\nabla}_y - \frac{e}{c} \widetilde{A}_y \\ &= \frac{\hbar}{i} \frac{\nabla_y}{2} - p - \frac{e}{c} \widetilde{A}_y. \end{aligned}$$

Let us take

$$\widehat{w} = \begin{pmatrix} w_{1,1} \\ w_{1,2} \\ w_{2,1} \\ w_{2,2} \end{pmatrix} \tag{12}$$

by equality (2.6), if

$$-\frac{ei}{\hbar} \Theta_-(\phi) w + \frac{ei}{4mc} \left[\Theta_-(B^i) [\sigma_i, w]_+ + \Theta_+(B^i) [\sigma_i, w]_- \right] = 0 \tag{13}$$

we get

$$\partial_t \widehat{w} = -\frac{1}{m} \mathcal{D} \mathcal{P} \widehat{w} \tag{14}$$

where

$$\mathcal{D} = -\widetilde{\mathcal{P}}_r \widehat{\mathbf{1}} \tag{15}$$

and

$$\mathcal{P} = \widetilde{\mathcal{P}}_p \widehat{\mathbf{1}} \tag{16}$$

$$\text{with } \widehat{\mathbf{1}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Moreover, by (10), (15) and (16), we obtain

$$\partial_t \widehat{w} = -\frac{1}{m} \mathcal{D} \mathcal{P} \widehat{w} + \Theta \widehat{w} \tag{17}$$

where $\Theta \widehat{w}$ is a potential pseudo-differential operator that we will see. We will consider the "local average" of any phase-space quantity f defin by

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

then for us $\langle \widehat{w} \rangle = \langle \widehat{w} \rangle (r) = \int_{\mathbb{R}^d} \widehat{w}(r, p) dp$.

For for the Pauli Hamiltonian with $\Theta \widehat{w} = 0$ we have the Wigner equation (17) and since the operator \mathcal{D} does not involve the momentum variable p , then $\langle \mathcal{D} \cdot \rangle = \mathcal{D} \langle \cdot \rangle$ and we get the order-0 moment equation

$$\partial_t \langle \widehat{w} \rangle + \frac{1}{m} \mathcal{D} \langle \mathcal{P} \widehat{w} \rangle = 0 \tag{18}$$

moreover, since \mathcal{D} and \mathcal{P} commute, we have the order-1 moment equation

$$\partial_t \langle \mathcal{P} \widehat{w} \rangle + \frac{1}{m} \mathcal{D} \langle \mathcal{P} \otimes \mathcal{P} \widehat{w} \rangle = 0 \tag{19}$$

and more in general the order-m moment equation

$$\partial_t \langle \mathcal{P}^{\otimes m} \widehat{w} \rangle + \frac{1}{m} \mathcal{D} \langle \mathcal{P}^{\otimes (m+1)} \widehat{w} \rangle = 0 \tag{20}$$

where $\mathcal{P}^{\otimes m} = \overbrace{\mathcal{P} \otimes \dots \otimes \mathcal{P}}^{m\text{-time}}$.

Remark 1. For the free Pauli Hamiltonian, from (17), with $\phi = 0$ and $A = B = 0$, we have

$$\partial_t \widehat{w} = -\frac{1}{m} \nabla_r \cdot p \widehat{w} \tag{21}$$

that it is the usual Wigner equation for free 1/2 spin particle.

Let us introduce the following notations:

$$n = \langle \widehat{w} \rangle \tag{22}$$

and

$$J = \langle \mathcal{P} \widehat{w} \rangle \tag{23}$$

then by (18), (22) and (23) we get

$$\partial_t n + \frac{1}{m} \mathcal{D} J = 0. \tag{24}$$

As in (L. Barletti, 2003) we use the following convention: every operation between colum-vectors has to be understood component-wise. For example we have

$$\begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix} = \begin{pmatrix} a_1 b_1 \\ a_2 b_2 \\ a_3 b_3 \\ a_4 b_4 \end{pmatrix} \tag{25}$$

and

$$\begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} / \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix} = \begin{pmatrix} a_1/b_1 \\ a_2/b_2 \\ a_3/b_3 \\ a_4/b_4 \end{pmatrix}; \tag{26}$$

moreover, if a_i, b_i are vectors (such as the for components of $\langle \mathcal{P}\widehat{w} \rangle$)

$$\begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} \cdot \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix} = \begin{pmatrix} a_1 \cdot b_1 \\ a_2 \cdot b_2 \\ a_3 \cdot b_3 \\ a_4 \cdot b_4 \end{pmatrix} \tag{27}$$

and

$$\begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} \otimes \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix} = \begin{pmatrix} a_1 \otimes b_1 \\ a_2 \otimes b_2 \\ a_3 \otimes b_3 \\ a_4 \otimes b_4 \end{pmatrix}. \tag{28}$$

Since $\widetilde{P}_x = \frac{\hbar}{i} \widetilde{\nabla}_x - \frac{e}{c} \widetilde{A}_x, \widetilde{P}_y = \frac{\hbar}{i} \widetilde{\nabla}_y - \frac{e}{c} \widetilde{A}_y$ and

$$\begin{aligned} \mathcal{D} &= \widetilde{\mathcal{P}}_r 1 = \mathcal{W} \left(\frac{P_x + P_y}{i\hbar} \right) \mathcal{W}^{-1} = \frac{\widetilde{P}_x + \widetilde{P}_y}{i\hbar} \\ \mathcal{P} &= \widetilde{\mathcal{P}}_p 1 = \mathcal{W} \left(\frac{P_x - P_y}{2} \right) \mathcal{W}^{-1} = \frac{\widetilde{P}_x - \widetilde{P}_y}{2} \end{aligned} \tag{29}$$

we obtain

$$\begin{aligned} \mathcal{P} \otimes \mathcal{P} = \mathcal{P}^{\otimes 2} &= \left(\frac{\widetilde{P}_x - \widetilde{P}_y}{2} \right)^{\otimes 2} \\ &= \frac{1}{4} \left(\widetilde{P}_x^{\otimes 2} + \widetilde{P}_y^{\otimes 2} - 2\widetilde{P}_x \otimes \widetilde{P}_y \right) \\ &= \frac{1}{4} \left(\widetilde{P}_x^{\otimes 2} + \widetilde{P}_y^{\otimes 2} + 2\widetilde{P}_x \otimes \widetilde{P}_y \right) - \widetilde{P}_x \otimes \widetilde{P}_y \\ &= \frac{1}{4} \left(\widetilde{P}_x + \widetilde{P}_y \right)^{\otimes 2} - \widetilde{P}_x \otimes \widetilde{P}_y \\ &= -\frac{\hbar^2}{4} \left(\frac{\widetilde{P}_x + \widetilde{P}_y}{i\hbar} \right)^{\otimes 2} - \widetilde{P}_x \otimes \widetilde{P}_y \\ &= -\frac{\hbar^2}{4} \mathcal{D}^{\otimes 2} - \widetilde{P}_x \otimes \widetilde{P}_y \end{aligned} \tag{30}$$

where the component-wise commutativity between \widetilde{P}_x and \widetilde{P}_y was used. Moreover we get

$$\langle \mathcal{P}^{\otimes 2} \widehat{w} \rangle = -\frac{\hbar^2}{4} \mathcal{D}^{\otimes 2} \langle \widehat{w} \rangle - \langle \widetilde{P}_x \otimes \widetilde{P}_y \widehat{w} \rangle \tag{31}$$

and

$$\begin{aligned} \langle \mathcal{P}\widehat{w} \rangle^{\otimes 2} &= \left\langle \frac{\widetilde{P}_x - \widetilde{P}_y}{2} \widehat{w} \right\rangle^{\otimes 2} \\ &= \frac{1}{4} \left(\langle \widetilde{P}_x \widehat{w} \rangle^{\otimes 2} + \langle \widetilde{P}_y \widehat{w} \rangle^{\otimes 2} - 2 \langle \widetilde{P}_x \widehat{w} \rangle \otimes \langle \widetilde{P}_y \widehat{w} \rangle \right) \\ &= \frac{1}{4} \langle \widetilde{P}_x + \widetilde{P}_y \widehat{w} \rangle^{\otimes 2} - \langle \widetilde{P}_x \widehat{w} \rangle \otimes \langle \widetilde{P}_y \widehat{w} \rangle \\ &= -\frac{\hbar^2}{4} \langle \mathcal{D}\widehat{w} \rangle^{\otimes 2} - \langle \widetilde{P}_x \widehat{w} \rangle \otimes \langle \widetilde{P}_y \widehat{w} \rangle \\ &= -\frac{\hbar^2}{4} (\mathcal{D} \langle \widehat{w} \rangle)^{\otimes 2} - \langle \widetilde{P}_x \widehat{w} \rangle \otimes \langle \widetilde{P}_y \widehat{w} \rangle \\ &= -\frac{\hbar^2}{4} (\mathcal{D} \langle \widehat{w} \rangle) \otimes (\mathcal{D} \langle \widehat{w} \rangle) - \langle \widetilde{P}_x \widehat{w} \rangle \otimes \langle \widetilde{P}_y \widehat{w} \rangle \end{aligned} \tag{32}$$

then

$$\langle \mathcal{P} \otimes P\widehat{w} \rangle = \frac{J \otimes J}{n} + Q(n) - nT \tag{33}$$

where

$$Q(n) = -\frac{\hbar^2}{4} \left((\mathcal{D} \otimes \mathcal{D})n - \frac{(\mathcal{D}n) \otimes (\mathcal{D}n)}{n} \right) \tag{34}$$

and

$$nT = \langle \widetilde{P}_x \otimes \widetilde{P}_y \widehat{w} \rangle - \frac{\langle \widetilde{P}_x \widehat{w} \rangle \otimes \langle \widetilde{P}_y \widehat{w} \rangle}{n}. \tag{35}$$

Proposition 1. Let $w = \mathcal{W}_Q$ 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; then

$$T = \sum_{s=1}^{+\infty} \frac{\lambda_s n^s}{n} \left(\frac{\langle \widetilde{\mathcal{P}}_x \widehat{w}^s \rangle}{n^s} - \frac{\langle \widetilde{\mathcal{P}}_x \widehat{w} \rangle}{n} \right) \otimes \left(\frac{\langle \widetilde{\mathcal{P}}_x \widehat{w}^s \rangle}{(n^s)^*} - \frac{\langle \widetilde{\mathcal{P}}_x \widehat{w} \rangle}{(n)^*} \right)^* \tag{36}$$

where $\widehat{w}^s = \mathcal{W}_{\varrho^s}$, $n^s = \langle w^s \rangle$ and $*$ denotes adjunction:

$$\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}^* = \begin{pmatrix} \bar{a} \\ \bar{b} \\ \bar{c} \\ \bar{d} \end{pmatrix}.$$

Proof. Let us define

$$q = \langle \widetilde{\mathcal{P}}_x \widehat{w} \rangle = \langle P_x \varrho \rangle \tag{37}$$

and

$$q^s = \langle \widetilde{\mathcal{P}}_x \widehat{w}^s \rangle \tag{38}$$

then

$$q = \langle P_x \varrho \rangle = \sum_{s=1}^{+\infty} \lambda_s q_s. \tag{39}$$

Since $\langle P_x \varrho \rangle = \langle P_y \varrho \rangle^*$, for a pure state, we have

$$\langle \widetilde{\mathcal{P}}_x \otimes \widetilde{\mathcal{P}}_y \widehat{w}^s \rangle = \frac{q^s \otimes (q^s)^*}{n^s} \tag{40}$$

From (35) and (40) we get

$$\begin{aligned} T &= \frac{1}{n} \left\langle \widetilde{\mathcal{P}}_x \otimes \widetilde{\mathcal{P}}_y \widehat{w} \right\rangle - \frac{\langle \widetilde{\mathcal{P}}_x \widehat{w} \rangle \otimes \langle \widetilde{\mathcal{P}}_y \widehat{w} \rangle}{n^2} \\ &= \sum_{s=1}^{+\infty} \lambda_s \frac{\langle \widetilde{\mathcal{P}}_x \otimes \widetilde{\mathcal{P}}_y \widehat{w}^s \rangle}{n} - \frac{\langle \widetilde{\mathcal{P}}_x \widehat{w} \rangle \otimes \langle \widetilde{\mathcal{P}}_y \widehat{w} \rangle}{n^2} \\ &= \sum_{s=1}^{+\infty} b^s \frac{q^s}{n^s} \otimes \frac{(q^s)^*}{n^s} - \frac{\langle \widetilde{\mathcal{P}}_x \widehat{w} \rangle \otimes \langle \widetilde{\mathcal{P}}_y \widehat{w} \rangle}{n^2} \end{aligned} \tag{41}$$

where

$$b^s = \frac{\lambda_s n^s}{n}. \tag{42}$$

Since

$$\begin{aligned} \sum_{s=1}^{+\infty} b^s \left(\frac{q^s}{n^s} - \frac{q}{n} \right) \otimes \left(\frac{q^s}{(n^s)^*} - \frac{q}{(n)^*} \right)^* &= \sum_{s=1}^{+\infty} b^s \left(\frac{q^s}{n^s} - \frac{q}{n} \right) \otimes \left(\left(\frac{q^s}{(n^s)^*} \right)^* - \left(\frac{q}{(n)^*} \right)^* \right) \\ &= \sum_{s=1}^{+\infty} b^s \left(\frac{q^s}{n^s} \otimes \left(\frac{q^s}{(n^s)^*} \right)^* - \frac{q^s}{n^s} \otimes \left(\frac{q}{(n)^*} \right)^* \right) + \\ &\quad + \sum_{s=1}^{+\infty} b^s \left(-\frac{q}{n} \otimes \left(\frac{q^s}{(n^s)^*} \right)^* + \frac{q}{n} \otimes \left(\frac{q}{(n)^*} \right)^* \right) \\ &= \sum_{s=1}^{+\infty} b^s \frac{q^s}{n^s} \otimes \left(\frac{q^s}{(n^s)^*} \right)^* - \left(\sum_{s=1}^{+\infty} b^s \frac{q^s}{n^s} \right) \otimes \left(\frac{q}{(n)^*} \right)^* - \\ &\quad - \frac{q}{n} \otimes \left(\sum_{s=1}^{+\infty} b^s \left(\frac{q^s}{(n^s)^*} \right)^* \right) + \frac{q}{n} \otimes \left(\frac{q}{(n)^*} \right)^* \end{aligned} \tag{43}$$

and

$$\begin{aligned} \sum_{s=1}^{+\infty} b^s \frac{q^s}{n^s} &= \frac{q}{n} \\ \sum_{s=1}^{+\infty} b^s \left(\frac{q^s}{(n^s)^*} \right)^* &= \sum_{s=1}^{+\infty} \frac{\lambda_s}{n} (q^s)^* = \frac{1}{n} (q)^* \end{aligned} \tag{44}$$

we get

$$\begin{aligned}
 \sum_{s=1}^{+\infty} b^s \left(\frac{q^s}{n^s} - \frac{q}{n} \right) \otimes \left(\frac{q^s}{(n^s)^*} - \frac{q}{(n)^*} \right)^* &= \sum_{s=1}^{+\infty} b^s \frac{q^s}{n^s} \otimes \left(\frac{q^s}{n^s} \right)^* - \frac{q}{n} \otimes \left(\frac{q}{n} \right)^* - \frac{q}{n} \otimes \frac{(q)^*}{n} + \frac{q}{n} \otimes \left(\frac{q}{n} \right)^* \\
 &= \sum_{s=1}^{+\infty} b^s \frac{q^s}{n^s} \otimes \left(\frac{q^s}{(n^s)^*} \right)^* - \frac{q}{n} \otimes \frac{(q)^*}{n} \\
 &= \sum_{s=1}^{+\infty} b^s \frac{q^s}{n^s} \otimes \frac{(q^s)^*}{n^s} - \frac{\langle \tilde{\mathcal{P}}_x \tilde{w} \rangle \langle \tilde{\mathcal{P}}_y \tilde{w} \rangle}{n^2} \\
 &= T.
 \end{aligned} \tag{45}$$

□

Corollary 1. *If $w = \mathcal{W}_Q$ is the Wigner transform of a pure-state density matrix, then $T = 0$.*

From (37) we get

$$\begin{aligned}
 q &= \langle \tilde{\mathcal{P}}_x \tilde{w} \rangle \\
 &= \left\langle \left[\left(\frac{\tilde{\mathcal{P}}_x - \tilde{\mathcal{P}}_y}{2} \right) + \left(\frac{\tilde{\mathcal{P}}_x + \tilde{\mathcal{P}}_y}{2} \right) \right] \tilde{w} \right\rangle \\
 &= \left\langle \left(\frac{\tilde{\mathcal{P}}_x - \tilde{\mathcal{P}}_y}{2} \right) \tilde{w} \right\rangle + \frac{i\hbar}{2} \left\langle \left(\frac{\tilde{\mathcal{P}}_x + \tilde{\mathcal{P}}_y}{i\hbar} \right) \tilde{w} \right\rangle \\
 &= \langle \mathcal{P} \tilde{w} \rangle + \frac{i\hbar}{2} \langle \mathcal{D} \tilde{w} \rangle \\
 &= J + \frac{i\hbar}{2} \mathcal{D}n
 \end{aligned} \tag{46}$$

and $q^s = J^s + \frac{i\hbar}{2} \mathcal{D}n^s$, with $J^s = \langle \mathcal{P} \tilde{w}^s \rangle$, then

$$\begin{aligned}
 T &= \sum_{s=1}^{+\infty} b^s \left(\frac{q^s}{n^s} - \frac{q}{n} \right) \otimes \left(\frac{q^s}{(n^s)^*} - \frac{q}{(n)^*} \right)^* \\
 &= \sum_{s=1}^{+\infty} b^s \left(\frac{J^s + \frac{i\hbar}{2} \mathcal{D}n^s}{n^s} - \frac{J + \frac{i\hbar}{2} \mathcal{D}n}{n} \right) \otimes \left(\frac{J^s + \frac{i\hbar}{2} \mathcal{D}n^s}{(n^s)^*} - \frac{J + \frac{i\hbar}{2} \mathcal{D}n}{(n)^*} \right)^* \\
 &= \sum_{s=1}^{+\infty} b^s \left(\frac{J^s}{n^s} - \frac{J}{n} \right) \otimes \left(\frac{J^s}{(n^s)^*} - \frac{J}{(n)^*} \right)^* + \\
 &\quad - \frac{i\hbar}{2} \sum_{s=1}^{+\infty} b^s \left(\frac{J^s}{n^s} - \frac{J}{n} \right) \otimes \left(\frac{\mathcal{D}n^s}{(n^s)^*} - \frac{\mathcal{D}n}{(n)^*} \right)^* + \\
 &\quad + \frac{i\hbar}{2} \sum_{s=1}^{+\infty} b^s \left(\frac{\mathcal{D}n^s}{n^s} - \frac{\mathcal{D}n}{n} \right) \otimes \left(\frac{J^s}{(n^s)^*} - \frac{J}{(n)^*} \right)^* + \\
 &\quad + \frac{\hbar^2}{4} \sum_{s=1}^{+\infty} b^s \left(\frac{\mathcal{D}n^s}{n^s} - \frac{\mathcal{D}n}{n} \right) \otimes \left(\frac{\mathcal{D}n^s}{(n^s)^*} - \frac{\mathcal{D}n}{(n)^*} \right)^*
 \end{aligned} \tag{47}$$

By decomposition (46) and (47) we have

$$T = T_c + T_{os} \tag{48}$$

where

$$T_c = \sum_{s=1}^{+\infty} b^s \left(\frac{J^s}{n^s} - \frac{J}{n} \right) \otimes \left(\frac{J^s}{(n^s)^*} - \frac{J}{(n)^*} \right)^* \tag{49}$$

is a "gauge-current temperature" and

$$T_{os} = \frac{\hbar^2}{4} \sum_{s=1}^{+\infty} b^s \left(\frac{\mathcal{D}n^s}{n^s} - \frac{\mathcal{D}n}{n} \right) \otimes \left(\frac{\mathcal{D}n^s}{(n^s)^*} - \frac{\mathcal{D}n}{(n)^*} \right)^* \tag{50}$$

is an "gauge-osmotic temperature".

From (20), (24) and (33) we obtain

$$\partial_t J + \frac{1}{m} \mathcal{D} \left(\frac{J \otimes J}{n} + Q(n) + nT \right) = 0. \tag{51}$$

Moreover, for $T = 0$, the system

$$\begin{cases} \partial_t n + \frac{1}{m} \mathcal{D}J = 0 \\ \partial_t J + \frac{1}{m} \mathcal{D} \left(\frac{J \otimes J}{n} + Q(n) \right) = 0 \end{cases} \tag{52}$$

it is a closed system of Madelung-like QHD equations for a free Pauli Hamiltonian.

2.1 Moments of the Potential Terms

In the following we will using a multi-index notation: a multi-index $\alpha = (\alpha_1, \dots, \alpha_N)$ is a -uple of non negative integer and $|\alpha| = \alpha_1 + \dots + \alpha_N$, $\alpha! = \alpha_1! \dots \alpha_N!$; moreover $\alpha \leq \beta$ if and only if $\alpha_i \leq \beta_i$ for $i = 1, \dots, N$.

Let us consider

$$\partial_t w = \frac{1}{m} \widetilde{P}_r \widetilde{P}_p w + V w \tag{53}$$

where

$$V w = -\frac{ei}{\hbar} \Theta_-(\phi) w + \frac{ei}{4mc} [\Theta_-(B^i) [\sigma_i, w]_+ + \Theta_+(B^i) [\sigma_i, w]_-] \tag{54}$$

since

$$[\sigma_1, w]_{\pm} = \begin{pmatrix} \pm\sigma_1 & 1 \\ 1 & \pm\sigma_1 \end{pmatrix} \widehat{w} = W_1^{\pm} \widehat{w}, \tag{55}$$

$$[\sigma_2, w]_{\pm} = \begin{pmatrix} \mp\sigma_2 & -i1 \\ i1 & \mp\sigma_2 \end{pmatrix} \widehat{w} = W_2^{\pm} \widehat{w} \tag{56}$$

and

$$[\sigma_3, w]_{\pm} = W_3^{\pm} \widehat{w} \tag{57}$$

with

$$W_3^+ = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 \end{pmatrix} \tag{58}$$

and

$$W_3^- = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}; \tag{59}$$

from (55), (56), (57), (58) and (59) we get

$$\partial_t \widehat{w} = -\frac{1}{m} \mathcal{D} \mathcal{P} \widehat{w} + \Theta \widehat{w} \tag{60}$$

where

$$\begin{aligned} \Theta \widehat{w} = & -\frac{ei}{\hbar} \Theta_-(\phi) \widehat{w} + \\ & + \frac{ei}{4mc} [\Theta_-(B^1) W_1^+ + \Theta_+(B^1) W_1^-] \widehat{w} + \\ & + \frac{ei}{4mc} [\Theta_-(B^2) W_2^+ + \Theta_+(B^2) W_2^-] \widehat{w} + \\ & + \frac{ei}{4mc} [\Theta_-(B^3) W_3^+ + \Theta_+(B^3) W_3^-] \widehat{w}. \end{aligned} \tag{61}$$

We define

$$I_1 = -\frac{ei}{\hbar} \begin{pmatrix} \Theta_-(\phi) & & & \\ & \Theta_-(\phi) & & \\ & & \Theta_-(\phi) & \\ & & & \Theta_-(\phi) \end{pmatrix} + \frac{ei}{2mc} \begin{pmatrix} \Theta_-(B^3) & 0 & 0 & 0 \\ 0 & \Theta_+(B^3) & 0 & 0 \\ 0 & 0 & -\Theta_+(B^3) & 0 \\ 0 & 0 & 0 & -\Theta_-(B^3) \end{pmatrix} \tag{62}$$

and

$$\begin{aligned}
 I_2 = & \frac{ei}{4mc} \left\{ (\Theta_-(B^1) - \Theta_+(B^1)) \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_1 \end{pmatrix} - \right. \\
 & - (\Theta_-(B^2) - \Theta_+(B^2)) \begin{pmatrix} \sigma_2 & 0 \\ 0 & \sigma_2 \end{pmatrix} + \\
 & + (\Theta_-(B^1) + \Theta_+(B^1)) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \\
 & \left. + (\Theta_-(B^2) + \Theta_+(B^2)) \begin{pmatrix} 0 & -i1 \\ i1 & 0 \end{pmatrix} \right\}.
 \end{aligned} \tag{63}$$

Let us consider the expansion of the pseudo-differential operator in a formal Taylor series with respect to $i\hbar\nabla_p$:

$$\tilde{\phi} \left(r \pm \frac{i\hbar}{2} \nabla_p \right) = \sum_{k=0}^{+\infty} \sum_{|\alpha|=k} \left(\pm \frac{i\hbar}{2} \right)^k \frac{\nabla^\alpha \phi(r)}{\alpha!} \nabla_p^\alpha, \tag{64}$$

let us consider

$$\begin{aligned}
 \mathbb{I}_1^1 &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} & \mathbb{I}_1^2 &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\
 \mathbb{I}_2^1 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} & \mathbb{I}_2^2 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}
 \end{aligned} \tag{65}$$

then we get

$$-\frac{ei}{\hbar} \Theta_-(\phi) \mathbf{1} = -\frac{ei}{\hbar} \sum_{k=0}^{+\infty} \sum_{|\alpha|=k} \sum_{j=1,2} \left(\frac{i\hbar}{2} \right)^k \frac{\nabla^\alpha \phi(r)}{\alpha!} \mathbb{H}_j^k \nabla_p^\alpha \tag{66}$$

where

$$\mathbb{H}_j^k = \mathbb{I}_j^1 - (-1)^k \mathbb{I}_j^2 \tag{67}$$

for $j = 1, 2$ and $k = 0, 1, \dots$

Let us consider

$$\begin{aligned}
 \mathbb{J}_1^1 &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} & \mathbb{J}_1^2 &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\
 \mathbb{J}_2^1 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} & \mathbb{J}_2^2 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}
 \end{aligned} \tag{68}$$

then

$$\begin{aligned}
 & \frac{ei}{2mc} \begin{pmatrix} \Theta_-(B^3) & 0 & 0 & 0 \\ 0 & \Theta_+(B^3) & 0 & 0 \\ 0 & 0 & -\Theta_+(B^3) & 0 \\ 0 & 0 & 0 & -\Theta_-(B^3) \end{pmatrix} = \\
 & = \frac{ei}{2mc} \sum_{k=0}^{+\infty} \sum_{|\alpha|=k} \sum_{j=1,2} \left(\frac{i\hbar}{2} \right)^k \frac{\nabla^\alpha B^3(r)}{\alpha!} \mathbb{Y}_j^k \nabla_p^\alpha
 \end{aligned} \tag{69}$$

where

$$\mathbb{Y}_j^k = \mathbb{J}_j^1 - (-1)^k \mathbb{J}_j^2 \tag{70}$$

for $j = 1, 2$ and $k = 0, 1, \dots$

From (66) and (69) we get

$$\begin{aligned} \langle \mathcal{P}^{\otimes n} I_1 \widehat{w} \rangle &= -\frac{ei}{\hbar} \sum_{k=0}^{+\infty} \sum_{|\alpha|=k} \sum_{j=1,2} \left(\frac{i\hbar}{2}\right)^k \frac{\nabla^\alpha \phi(r)}{\alpha!} \left\langle (p\mathbf{1})^{\otimes n} \mathbb{H}_j^k \nabla_p^\alpha \widehat{w} \right\rangle + \\ &+ \frac{ei}{2mc} \sum_{k=0}^{+\infty} \sum_{|\alpha|=k} \sum_{j=1,2} \left(\frac{i\hbar}{2}\right)^k \frac{\nabla^\alpha B^3(r)}{\alpha!} \left\langle (p\mathbf{1})^{\otimes n} \mathbb{Y}_j^k \nabla_p^\alpha \widehat{w} \right\rangle. \end{aligned} \tag{71}$$

Let us consider

$$\begin{aligned} \mathbb{N}_1 &= \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} & \mathbb{N}_2 &= \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix} \\ \mathbb{N}_3 &= \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} & \mathbb{N}_4 &= \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \end{aligned} \tag{72}$$

then

$$\begin{aligned} \langle \mathcal{P}^{\otimes n} I_2 \widehat{w} \rangle &= \frac{ei}{2mc} \left\{ -\sum_{k=0}^{+\infty} \sum_{|\alpha|=k} \left(-\frac{i\hbar}{2}\right)^k \frac{\nabla^\alpha B^1(r)}{\alpha!} \left\langle (p\mathbf{1})^{\otimes n} \mathbb{N}_1^k \nabla_p^\alpha \widehat{w} \right\rangle + \right. \\ &+ \sum_{k=0}^{+\infty} \sum_{|\alpha|=k} \left(-\frac{i\hbar}{2}\right)^k \frac{\nabla^\alpha B^2(r)}{\alpha!} \left\langle (p\mathbf{1})^{\otimes n} \mathbb{N}_2^k \nabla_p^\alpha \widehat{w} \right\rangle + \\ &+ \sum_{k=0}^{+\infty} \sum_{|\alpha|=k} \left(\frac{i\hbar}{2}\right)^k \frac{\nabla^\alpha B^1(r)}{\alpha!} \left\langle (p\mathbf{1})^{\otimes n} \mathbb{N}_3^k \nabla_p^\alpha \widehat{w} \right\rangle + \\ &\left. + \sum_{k=0}^{+\infty} \sum_{|\alpha|=k} \left(\frac{i\hbar}{2}\right)^k \frac{\nabla^\alpha B^2(r)}{\alpha!} \left\langle (p\mathbf{1})^{\otimes n} \mathbb{N}_4^k \nabla_p^\alpha \widehat{w} \right\rangle \right\} \end{aligned} \tag{73}$$

where

$$\mathbb{N}_j^k = \mathbb{N}_j \tag{74}$$

for $j = 1, 2, 3, 4$ and $k = 0, 1, \dots$

If we consider a single component $(p\mathbf{1})^\beta$ of the tensor product $(p\mathbf{1})^{\otimes n}$, where β is a multi-index with $|\beta| = n$, integration by parts yields

$$\begin{aligned} \left\langle (p\mathbf{1})^\beta \mathbb{H}_j^k \nabla_p^\alpha \widehat{w} \right\rangle &= \begin{cases} (-1)^k \left\langle (p\mathbf{1})^{\beta-\alpha} \mathbb{H}_j^k \widehat{w} \right\rangle & \text{if } \alpha \leq \beta \\ 0 & \text{if } \alpha \not\leq \beta \end{cases} \\ \left\langle (p\mathbf{1})^\beta \mathbb{Y}_j^k \nabla_p^\alpha \widehat{w} \right\rangle &= \begin{cases} (-1)^k \left\langle (p\mathbf{1})^{\beta-\alpha} \mathbb{Y}_j^k \widehat{w} \right\rangle & \text{if } \alpha \leq \beta \\ 0 & \text{if } \alpha \not\leq \beta \end{cases} \\ \left\langle (p\mathbf{1})^\beta \mathbb{N}_s^k \nabla_p^\alpha \widehat{w} \right\rangle &= \begin{cases} (-1)^k \left\langle (p\mathbf{1})^{\beta-\alpha} \mathbb{N}_s^k \widehat{w} \right\rangle & \text{if } \alpha \leq \beta \\ 0 & \text{if } \alpha \not\leq \beta \end{cases} \end{aligned} \tag{75}$$

for $j = 1, 2, s = 1, 2, 3, 4$ and $k = 0, 1, \dots$

From (71), (73) and (75) we get

$$\begin{aligned} \langle \mathcal{P}^{\otimes n} I_1 \widehat{w} \rangle &= -\frac{ei}{\hbar} \sum_{k=0}^n \sum_{|\alpha|=k} \sum_{j=1,2} \left(-\frac{i\hbar}{2}\right)^k \frac{\nabla^\alpha \phi(r)}{\alpha!} \left\langle \mathcal{P}^{\otimes n-\alpha} \mathbb{H}_j^k \widehat{w} \right\rangle + \\ &+ \frac{ei}{2mc} \sum_{k=0}^n \sum_{|\alpha|=k} \sum_{j=1,2} \left(-\frac{i\hbar}{2}\right)^k \frac{\nabla^\alpha B^3(r)}{\alpha!} \left\langle \mathcal{P}^{\otimes n-\alpha} \mathbb{Y}_j^k \widehat{w} \right\rangle \end{aligned} \tag{76}$$

and

$$\begin{aligned} \langle \mathcal{P}^{\otimes n} I_2 \widehat{w} \rangle &= -\frac{ei}{2mc} \sum_{k=0}^n \sum_{|\alpha|=k} \left(\frac{i\hbar}{2}\right)^k \frac{\nabla^\alpha B^1(r)}{\alpha!} \left\langle \mathcal{P}^{\otimes n-\alpha} \mathbb{N}_1^k \widehat{w} \right\rangle + \\ &+ \frac{ei}{2mc} \sum_{k=0}^n \sum_{|\alpha|=k} \left(\frac{i\hbar}{2}\right)^k \frac{\nabla^\alpha B^2(r)}{\alpha!} \left\langle \mathcal{P}^{\otimes n-\alpha} \mathbb{N}_2^k \widehat{w} \right\rangle + \\ &+ \frac{ei}{2mc} \sum_{k=0}^n \sum_{|\alpha|=k} \left(-\frac{i\hbar}{2}\right)^k \frac{\nabla^\alpha B^1(r)}{\alpha!} \left\langle \mathcal{P}^{\otimes n-\alpha} \mathbb{N}_3^k \widehat{w} \right\rangle \\ &+ \frac{ei}{2mc} \sum_{k=0}^n \sum_{|\alpha|=k} \left(-\frac{i\hbar}{2}\right)^k \frac{\nabla^\alpha B^2(r)}{\alpha!} \left\langle \mathcal{P}^{\otimes n-\alpha} \mathbb{N}_4^k \widehat{w} \right\rangle \end{aligned} \tag{77}$$

3. One-band Madelung Equations

Proposition (1) and corollary (1) imply that the $n = 0$ and $n = 1$ moment equations for a pure state are closed and yield a analogue of QHD Madelung equations.

For $n = 0$ we get:

$$\begin{aligned}
 \langle \Theta \widehat{w} \rangle &= -\frac{ei}{\hbar} \phi(r) \sum_{j=1,2} \langle \mathbb{H}_j^0 \widehat{w} \rangle + \frac{ei}{2mc} B^3(r) \sum_{j=1,2} \langle \mathbb{Y}_j^0 \widehat{w} \rangle - \\
 &\quad - \frac{ei}{2mc} B^1(r) \langle \mathbb{N}_1^0 \widehat{w} \rangle + \frac{ei}{2mc} B^2(r) \langle \mathbb{N}_2^0 \widehat{w} \rangle + \\
 &\quad + \frac{ei}{2mc} B^1(r) \langle \mathbb{N}_3^0 \widehat{w} \rangle + \frac{ei}{2mc} B^2(r) \langle \mathbb{N}_4^0 \widehat{w} \rangle \\
 &= \frac{ei}{2mc} B^1(r) \mathbb{M}_1 \langle \widehat{w} \rangle + \frac{ei}{2mc} B^2(r) \mathbb{M}_2 \langle \widehat{w} \rangle
 \end{aligned} \tag{78}$$

where

$$\mathbb{M}_1 = \begin{pmatrix} 0 & -1 & 0 & 1 \\ -1 & 0 & 1 & 0 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & -1 & 0 \end{pmatrix} \quad \mathbb{M}_2 = \begin{pmatrix} 0 & -i & 0 & -i \\ i & 0 & -i & 0 \\ 0 & i & 0 & -i \\ i & 0 & i & 0 \end{pmatrix} \tag{79}$$

For $n = 1$ we get:

if $k = 0$

$$\begin{aligned}
 -\frac{ei}{\hbar} \sum_{j=1,2} \phi(r) \langle \mathcal{P} \mathbb{H}_j^0 \widehat{w} \rangle &= -\frac{ei}{\hbar} \sum_{j=1,2} \phi(r) \mathbb{H}_j^0 \langle \mathcal{P} \widehat{w} \rangle \\
 \frac{ei}{2mc} \sum_{j=1,2} B^3(r) \langle \mathcal{P} \mathbb{Y}_j^0 \widehat{w} \rangle &= \frac{ei}{2mc} \sum_{j=1,2} B^3(r) \mathbb{Y}_j^0 \langle \mathcal{P} \widehat{w} \rangle \\
 \frac{-ei}{2mc} B^1(r) \langle \mathcal{P} \mathbb{N}_1 \widehat{w} \rangle &= \frac{-ei}{2mc} B^1(r) \mathbb{N}_1 \langle \mathcal{P} \widehat{w} \rangle \\
 \frac{ei}{2mc} B^2(r) \langle \mathcal{P} \mathbb{N}_2 \widehat{w} \rangle &= \frac{ei}{2mc} B^2(r) \mathbb{N}_2 \langle \mathcal{P} \widehat{w} \rangle \\
 \frac{ei}{2mc} B^1(r) \langle \mathcal{P} \mathbb{N}_3 \widehat{w} \rangle &= \frac{ei}{2mc} B^1(r) \mathbb{N}_3 \langle \mathcal{P} \widehat{w} \rangle \\
 \frac{ei}{2mc} B^2(r) \langle \mathcal{P} \mathbb{N}_4 \widehat{w} \rangle &= \frac{ei}{2mc} B^2(r) \mathbb{N}_4 \langle \mathcal{P} \widehat{w} \rangle
 \end{aligned} \tag{80}$$

and

$$\begin{aligned}
 \mathbb{G}J &= \left[-\frac{ei}{\hbar} \sum_{j=1,2} \phi(r) \mathbb{H}_j^0 + \frac{ei}{2mc} \sum_{j=1,2} B^3(r) \mathbb{Y}_j^0 - \right. \\
 &\quad \left. - \frac{ei}{2mc} B^1(r) \mathbb{N}_1 + \frac{ei}{2mc} B^2(r) \mathbb{N}_2 + \frac{ei}{2mc} B^1(r) \mathbb{N}_3 + \frac{ei}{2mc} B^2(r) \mathbb{N}_4 \right] \langle \mathcal{P} \widehat{w} \rangle;
 \end{aligned} \tag{81}$$

if $k = 1$ we get

$$\begin{aligned}
 -\frac{ei}{\hbar} \sum_{|\alpha|=1} \sum_{j=1,2} \left(-\frac{i\hbar}{2} \right) \nabla^\alpha \phi(r) \langle \mathbb{H}_j^1 \widehat{w} \rangle &= -\frac{e}{2} \sum_{|\alpha|=1} \sum_{j=1,2} \nabla^\alpha \phi(r) \mathbb{H}_j^1 \langle \widehat{w} \rangle \\
 \frac{ei}{2mc} \sum_{|\alpha|=1} \sum_{j=1,2} \left(-\frac{i\hbar}{2} \right) \frac{\nabla^\alpha B^3(r)}{\alpha!} \langle \mathbb{Y}_j^1 \widehat{w} \rangle &= \frac{e\hbar}{4mc} \sum_{|\alpha|=1} \sum_{j=1,2} \nabla^\alpha B^3(r) \mathbb{Y}_j^1 \langle \widehat{w} \rangle \\
 -\frac{ei}{2mc} \sum_{|\alpha|=1} \left(\frac{i\hbar}{2} \right) \frac{\nabla^\alpha B^1(r)}{\alpha!} \langle \mathbb{N}_1^1 \widehat{w} \rangle &= \frac{e\hbar}{4mc} \sum_{|\alpha|=1} \nabla^\alpha B^1(r) \mathbb{N}_1 \langle \widehat{w} \rangle \\
 \frac{ei}{2mc} \sum_{|\alpha|=1} \left(\frac{i\hbar}{2} \right) \frac{\nabla^\alpha B^2(r)}{\alpha!} \langle \mathbb{N}_2^1 \widehat{w} \rangle &= -\frac{e\hbar}{4mc} \sum_{|\alpha|=1} \nabla^\alpha B^2(r) \mathbb{N}_2 \langle \widehat{w} \rangle \\
 \frac{ei}{2mc} \sum_{|\alpha|=k} \left(\frac{i\hbar}{2} \right) \frac{\nabla^\alpha B^1(r)}{\alpha!} \langle \mathbb{N}_3^1 \widehat{w} \rangle &= -\frac{e\hbar}{4mc} \sum_{|\alpha|=1} \nabla^\alpha B^1(r) \mathbb{N}_3 \langle \widehat{w} \rangle \\
 \frac{ei}{2mc} \sum_{|\alpha|=k} \left(\frac{i\hbar}{2} \right) \frac{\nabla^\alpha B^2(r)}{\alpha!} \langle \mathbb{N}_4^1 \widehat{w} \rangle &= -\frac{e\hbar}{4mc} \sum_{|\alpha|=1} \nabla^\alpha B^2(r) \mathbb{N}_4 \langle \widehat{w} \rangle
 \end{aligned} \tag{82}$$

and

$$\begin{aligned}
 \mathbb{E}n &= \left[-\frac{e}{2} \sum_{|\alpha|=1} \sum_{j=1,2} \nabla^\alpha \phi(r) \mathbb{H}_j^1 + \frac{e\hbar}{4mc} \sum_{|\alpha|=1} \sum_{j=1,2} \nabla^\alpha B^3(r) \mathbb{Y}_j^1 - \right. \\
 &\quad \left. - \frac{e\hbar}{4mc} \sum_{|\alpha|=1} \nabla^\alpha B^1(r) \mathbb{N}_1 + \frac{e\hbar}{4mc} \sum_{|\alpha|=1} \nabla^\alpha B^2(r) \mathbb{N}_2 + \right. \\
 &\quad \left. + \frac{e\hbar}{4mc} \sum_{|\alpha|=1} \nabla^\alpha B^1(r) \mathbb{N}_3 + \frac{e\hbar}{4mc} \sum_{|\alpha|=1} \nabla^\alpha B^2(r) \mathbb{N}_4 \right] \langle \widehat{w} \rangle.
 \end{aligned} \tag{83}$$

Then we can write the moment equations for $n = 0$ and $n = 1$ in the following form:

$$\begin{cases} \partial_t n + \frac{1}{m} \mathcal{D}J = \frac{ei}{2mc} [B^1(r) \mathbb{M}_1 + B^2(r) \mathbb{M}_2] n \\ \partial_t J + \frac{1}{m} \mathcal{D} \left(\frac{J \otimes J}{n} + Q(n) + nT \right) = \mathbb{G}J + \mathbb{E}n \end{cases} \tag{84}$$

By Corollary (1) for a pure state we have $T = 0$, then

$$\begin{cases} \partial_t n + \frac{1}{m} \mathcal{D}J = \frac{e_i}{2mc} [B^1(r) \mathbb{M}_1 + B^2(r) \mathbb{M}_2] n \\ \partial_t J + \frac{1}{m} \mathcal{D} \left(\frac{J \otimes J}{n} + Q(n) \right) = \mathbb{G}J + \mathbb{E}n \end{cases} \tag{85}$$

is a closed Madelung-like system for a pure state.

4. A Two-band Kp Pauli Hamiltonian

Now we consider the following Hamiltonian:

$$H_{kp}^{\text{Pauli}} = \begin{pmatrix} \frac{1}{2m} \left(\frac{\hbar}{i} \nabla - \frac{e}{c} A \right)^2 \sigma_0 + V_1^j \sigma_j & \frac{K}{m} \left(\frac{\hbar}{i} \nabla - \frac{e}{c} A \right) \sigma_0 \\ -\frac{K}{m} \left(\frac{\hbar}{i} \nabla - \frac{e}{c} A \right) \sigma_0 & \frac{1}{2m} \left(\frac{\hbar}{i} \nabla - \frac{e}{c} A \right)^2 \sigma_0 + V_2^j \sigma_j \end{pmatrix} \tag{86}$$

where $K = \langle u_1 | \left(\frac{\hbar}{i} \nabla - \frac{e}{c} A \right) | u_2 \rangle$. The Hamiltonian (86) is the equivalent of the Hamiltonian (3) considering the electron as a particle. The Hamiltonian (86) describes an 1/2 spin electron that "sees" two energy bands available and a Zener tunneling between the two-band is possible. Let us take

$$P = \begin{pmatrix} \left(\frac{\hbar}{i} \nabla - \frac{e}{c} A \right) \sigma_0 & K \sigma_0 \\ -K \sigma_0 & \left(\frac{\hbar}{i} \nabla - \frac{e}{c} A \right) \sigma_0 \end{pmatrix} \tag{87}$$

then

$$P^2 = \begin{pmatrix} \left(\frac{\hbar}{i} \nabla - \frac{e}{c} A \right)^2 \sigma_0 & 2K \left(\frac{\hbar}{i} \nabla - \frac{e}{c} A \right) \sigma_0 \\ -2K \left(\frac{\hbar}{i} \nabla - \frac{e}{c} A \right) \sigma_0 & \left(\frac{\hbar}{i} \nabla - \frac{e}{c} A \right)^2 \sigma_0 \end{pmatrix} - K^2 \begin{pmatrix} \sigma_0 & 0 \\ 0 & \sigma_0 \end{pmatrix} \tag{88}$$

and

$$H_{kp}^{\text{Pauli}} = \frac{1}{2m} P^2 + \frac{K^2}{2m} \begin{pmatrix} \sigma_0 & 0 \\ 0 & \sigma_0 \end{pmatrix} + \begin{pmatrix} V_1^j \sigma_j & 0 \\ 0 & V_2^j \sigma_j \end{pmatrix}. \tag{89}$$

We put $p = \left(\frac{\hbar}{i} \nabla - \frac{e}{c} A \right)$ and we consider

$$H_{kp}^{\text{Pauli}} = \frac{1}{2m} p^2 \mathbf{1} - \frac{Kp}{m} W + V_1^j Z_j^1 + V_2^j Z_j^2 \tag{90}$$

where

$$W = \begin{pmatrix} 0 & -\sigma_0 \\ \sigma_0 & 0 \end{pmatrix}, Z_j^1 = \begin{pmatrix} \sigma_j & 0 \\ 0 & 0 \end{pmatrix}, Z_j^2 = \begin{pmatrix} 0 & 0 \\ 0 & \sigma_j \end{pmatrix} \tag{91}$$

then

$$\begin{aligned} i\hbar \partial_t \varrho &= \left[\frac{1}{2m} p_x^2 - \frac{1}{2m} p_y^2 \right] \varrho - \frac{k(p_x - p_y)}{2m} [W; \varrho]_+ - \frac{k(p_x + p_y)}{2m} [W; \varrho]_- + \\ &+ \frac{(V_1^j(x) - V_1^j(y))}{2} [Z_j^1; \varrho]_+ + \frac{(V_2^j(x) - V_2^j(y))}{2} [Z_j^2; \varrho]_+ + \\ &+ \frac{(V_1^j(x) + V_1^j(y))}{2} [Z_j^1; \varrho]_- + \frac{(V_2^j(x) + V_2^j(y))}{2} [Z_j^2; \varrho]_- . \end{aligned} \tag{92}$$

If $V_1^j = V_2^j = 0$, we get

$$i\hbar \partial_t \varrho = \left[\frac{1}{2m} p_x^2 - \frac{1}{2m} p_y^2 \right] \varrho - \frac{k(p_x - p_y)}{2m} [W; \varrho]_+ - \frac{k(p_x + p_y)}{2m} [W; \varrho]_- , \tag{93}$$

since

$$[W; \varrho]_{\pm} = \widehat{W}_{\pm} \widehat{\varrho} \tag{94}$$

where $\widehat{\varrho} = (\varrho_{1,1}, \dots, \varrho_{1,4}, \dots, \varrho_{4,1}, \dots, \varrho_{4,4})^t$ and

$$\widehat{W}_{\pm} = \begin{pmatrix} \mp W & 0 & -1 & 0 \\ 0 & \mp W & 0 & -1 \\ 1 & 0 & \mp W & 0 \\ 0 & 1 & 0 & \mp W \end{pmatrix}, \tag{95}$$

then equation (93) is equivalent to

$$i\hbar\partial_t\widehat{\rho} = \frac{(p_x^2 - p_y^2)}{2m}\widehat{\rho} - \frac{k(p_x - p_y)}{2m}\widehat{W}_+\widehat{\rho} - \frac{k(p_x + p_y)}{2m}\widehat{W}_-\widehat{\rho} \tag{96}$$

and

$$i\hbar\partial_t\widehat{\rho} = \frac{1}{2m} [(p_x - p_y)\widehat{1} - k\widehat{W}_-] [(p_x + p_y)\widehat{1} - k\widehat{W}_+] \widehat{\rho} - \frac{k^2}{2m}\widehat{W}_-\widehat{W}_+\widehat{\rho} \tag{97}$$

with $\widehat{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$; since $\widehat{W}_-\widehat{W}_+ = \widehat{1}$, we get

$$\partial_t\widehat{\rho} = \frac{1}{m} \left[\left(\frac{p_x - p_y}{2} \right) \widehat{1} - \frac{k}{2} \widehat{W}_- \right] \left[\left(\frac{p_x + p_y}{i\hbar} \right) \widehat{1} + \frac{ik}{\hbar} \widehat{W}_+ \right] \widehat{\rho} + \frac{ik^2}{2m\hbar} \widehat{\rho}. \tag{98}$$

Now we write the equation of evolution of the time-dependent Wigner matrix

$$\partial_t\widehat{w} = -\frac{1}{m}\mathcal{P}\mathcal{D}\widehat{w} + \frac{ik^2}{2m\hbar}\widehat{w} \tag{99}$$

where

$$\mathcal{P} = \left[\left(\frac{\widetilde{p}_x - \widetilde{p}_y}{2} \right) \widehat{1} - \frac{k}{2} \widehat{W}_- \right] \tag{100}$$

and

$$\mathcal{D} = - \left[\left(\frac{\widetilde{p}_x + \widetilde{p}_y}{i\hbar} \right) \widehat{1} + \frac{ik}{\hbar} \widehat{W}_+ \right], \tag{101}$$

with

$$\begin{cases} \widetilde{p}_x = \frac{\hbar}{i}\widetilde{\nabla}_x - \frac{e}{c}\widetilde{A}_x = \frac{\hbar}{i}\frac{\nabla_x}{2} + p - \frac{e}{c}\widetilde{A}_x \\ \widetilde{p}_y = \frac{\hbar}{i}\widetilde{\nabla}_y - \frac{e}{c}\widetilde{A}_y = \frac{\hbar}{i}\frac{\nabla_y}{2} - p - \frac{e}{c}\widetilde{A}_y \end{cases} \tag{102}$$

and

$$\begin{cases} \frac{\widetilde{p}_x - \widetilde{p}_y}{2} = p - \frac{e}{2c}\Theta_-(A) \\ \frac{\widetilde{p}_x + \widetilde{p}_y}{i\hbar} = -\nabla_r - \frac{e}{2c}\Theta_+(A) \end{cases}; \tag{103}$$

moreover

$$\mathcal{D} = \left[\nabla_r \widehat{1} + \frac{e}{2c}\Theta_+(A)\widehat{1} + \frac{ik}{\hbar}\widehat{W}_+ \right] \tag{104}$$

and

$$\mathcal{P} = \left[p\widehat{1} - \frac{e}{2c}\Theta_-(A)\widehat{1} - \frac{k}{2}\widehat{W}_- \right]. \tag{105}$$

From (100) and (101) we get

$$\mathcal{P}^{\otimes 2} = \frac{1}{4} \left[(\widetilde{p}_x - \widetilde{p}_y)^{\otimes 2} - 2k(\widetilde{p}_x - \widetilde{p}_y)\widehat{1} \otimes \widehat{W}_- + k^2\widehat{W}_- \otimes \widehat{W}_- \right] \tag{106}$$

and

$$\mathcal{D}^{\otimes 2} = \left[\left(\frac{\widetilde{p}_x + \widetilde{p}_y}{i\hbar} \right)^{\otimes 2} + 2\frac{ik^2}{\hbar} \left(\frac{\widetilde{p}_x + \widetilde{p}_y}{i\hbar} \right) \widehat{1} \otimes \widehat{W}_+ - \frac{k^2}{\hbar^2} \widehat{W}_+ \otimes \widehat{W}_+ \right] \tag{107}$$

then

$$\begin{aligned} \mathcal{P}^{\otimes 2} &= -\frac{\hbar^2}{4} \left(\frac{\widetilde{p}_x + \widetilde{p}_y}{i\hbar} \right)^{\otimes 2} - \widetilde{p}_x \otimes \widetilde{p}_y - \frac{k}{2} (\widetilde{p}_x - \widetilde{p}_y)\widehat{1} \otimes \widehat{W}_- + \frac{k^2}{4} \widehat{W}_- \otimes \widehat{W}_- \\ &= -\frac{\hbar^2}{4} \mathcal{D}^{\otimes 2} - \frac{i\hbar k}{2} \mathcal{D} \otimes \widehat{W}_+ - k\mathcal{P} \otimes \widehat{W}_- - \widetilde{p}_x \otimes \widetilde{p}_y + \frac{k^2}{4} [\widehat{W}_+^{\otimes 2} - \widehat{W}_-^{\otimes 2}] \end{aligned} \tag{108}$$

and, since $[\widehat{W}_+^2 - \widehat{W}_-^2] = 0$,

$$\langle \mathcal{P}^{\otimes 2} \widehat{w} \rangle = -\frac{\hbar^2}{4} \mathcal{D}^{\otimes 2} n - \frac{i\hbar k}{2} \widehat{W}_+ \mathcal{D} n - k\widehat{W}_- J - \langle \widetilde{p}_x \otimes \widetilde{p}_y \widehat{w} \rangle. \tag{109}$$

By (106), (107) and (108) we get

$$\begin{aligned} \langle \mathcal{P}\widehat{w} \rangle^{\otimes 2} &= \left\langle \left(\frac{\overline{p}_x - \overline{p}_y}{2} \right) \widehat{w} \right\rangle^{\otimes 2} - k \left\langle \left(\frac{\overline{p}_x - \overline{p}_y}{2} \right) \widehat{w} \right\rangle \otimes \langle \widehat{W}_- \widehat{w} \rangle + \frac{k^2}{4} \langle \widehat{W}_- \widehat{w} \rangle^{\otimes 2} \\ &= -\frac{\hbar^2}{4} \left\langle \left(\frac{\overline{p}_x + \overline{p}_y}{i\hbar} \right) \widehat{w} \right\rangle^{\otimes 2} - k \left\langle \left(\frac{\overline{p}_x - \overline{p}_y}{2} \right) \widehat{w} \right\rangle \otimes \langle \widehat{W}_- \widehat{w} \rangle + \frac{k^2}{4} \langle \widehat{W}_- \widehat{w} \rangle^{\otimes 2} + \\ &\quad + \langle \overline{p}_x \widehat{w} \rangle \otimes \langle \overline{p}_y \widehat{w} \rangle \end{aligned} \tag{110}$$

and

$$\langle \mathcal{D}\widehat{w} \rangle^{\otimes 2} = \left\langle \left(\frac{\overline{p}_x + \overline{p}_y}{i\hbar} \right) \widehat{w} \right\rangle^{\otimes 2} + \frac{2ik}{\hbar} \left\langle \left(\frac{\overline{p}_x + \overline{p}_y}{i\hbar} \right) \widehat{w} \right\rangle \otimes \langle \widehat{W}_+ \widehat{w} \rangle - \frac{k^2}{\hbar^2} \langle \widehat{W}_+ \widehat{w} \rangle^{\otimes 2}; \tag{111}$$

moreover by (108), (109) and (110) it follows that

$$\begin{aligned} \langle \mathcal{P}\widehat{w} \rangle^{\otimes 2} &= -\frac{\hbar^2}{4} (\mathcal{D}n)^{\otimes 2} + \langle \overline{p}_x \widehat{w} \rangle \otimes \langle \overline{p}_y \widehat{w} \rangle + \\ &\quad + \frac{i\hbar k}{2} (\mathcal{D}n) \otimes (\widehat{W}_+ n) - kJ \otimes (\widehat{W}_- n) + \frac{k^2}{4} \left[(\widehat{W}_+ n)^{\otimes 2} - (\widehat{W}_- n)^{\otimes 2} \right] \end{aligned} \tag{112}$$

then

$$\langle \mathcal{P} \otimes P\widehat{w} \rangle = \frac{J \otimes J}{n} + Q(n) + V(n) - nT \tag{113}$$

where

$$\begin{aligned} Q(n) &= -\frac{\hbar^2}{4} \left(\mathcal{D}^{2\otimes} n - \frac{(\mathcal{D}n)^{2\otimes}}{n} \right); \\ nT &= \langle \overline{\mathcal{P}}_x \otimes \overline{\mathcal{P}}_y \widehat{w} \rangle - \frac{\langle \overline{\mathcal{P}}_x \widehat{w} \rangle \otimes \langle \overline{\mathcal{P}}_y \widehat{w} \rangle}{n}; \\ V(n) &= k \left[\frac{J \otimes (\widehat{W}_- n)}{n} - \widehat{W}_- J \right] - \frac{i\hbar k}{2} \left[\frac{(\mathcal{D}n) \otimes (\widehat{W}_+ n)}{n} + \widehat{W}_+ \mathcal{D}n \right] - \frac{k^2}{4} \left[\frac{(\widehat{W}_+ n)^{\otimes 2}}{n} - \frac{(\widehat{W}_- n)^{\otimes 2}}{n} \right]. \end{aligned} \tag{114}$$

Proposition 2. Let $w = \mathcal{W}_Q$ 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; then

$$T = \sum_{s=1}^{+\infty} \frac{\lambda_s n^s}{n} \left(\frac{\langle \overline{p}_x \widehat{w}^s \rangle}{n^s} - \frac{\langle \overline{p}_x \widehat{w} \rangle}{n} \right) \otimes \left(\frac{\langle \overline{p}_x \widehat{w}^s \rangle}{(n^s)^*} - \frac{\langle \overline{p}_x \widehat{w} \rangle}{(n)^*} \right)^* \tag{115}$$

where $\widehat{w}^s = \mathcal{W}_{Q^s}$, $n^s = \langle w^s \rangle$ and $*$ denotes adjunction:

$$\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}^* = \begin{pmatrix} \bar{a} \\ \bar{b} \\ \bar{c} \\ \bar{d} \end{pmatrix}.$$

Corollary 2. If $w = \mathcal{W}_Q$ is the Wigner transform of a pure-state density matrix, then $T = 0$.

From (99) and (113) we obtain

$$\partial_t J + \frac{1}{m} \mathcal{D} \left(\frac{J \otimes J}{n} + Q(n) + nT - V(n) \right) - \frac{ik^2}{2m\hbar} J = 0 \tag{116}$$

and for $T = 0$

$$\begin{cases} \partial_t n + \frac{1}{m} \mathcal{D} J - \frac{ik^2}{2m\hbar} n = 0 \\ \partial_t J + \frac{1}{m} \mathcal{D} \left(\frac{J \otimes J}{n} + Q(n) - V(n) \right) - \frac{ik^2}{2m\hbar} J = 0 \end{cases} \tag{117}$$

is a closed system of Madelung-like QHD equations for a "free" two-band-gauge Kp Pauli Hamiltonian.

4.1 Moments of the Potential Terms

In the following we will using a multi-index notation: a multi-index $\alpha = (\alpha_1, \dots, \alpha_N)$ is a -uple of non negative integer and $|\alpha| = \alpha_1 + \dots + \alpha_N$, $\alpha! = \alpha_1! \dots \alpha_N!$; moreover $\alpha \leq \beta$ if and only if $\alpha_i \leq \beta_i$ for $i = 1, \dots, N$. For the potential we get

$$\left[Z_j^h, \varrho \right]_{\pm} = \mathbb{H}_{j,\pm}^h \widehat{Q} \tag{118}$$

where

$$\mathbb{H}_{j,\pm}^h = \pm \mathbb{Z}_{j,1}^h + \mathbb{Z}_{j,2}^h \tag{119}$$

for $h = 1, 2$ e $j = 1, 2, 3$.

By (118) and (119) we have

$$\begin{aligned} \frac{(V_h^j(x)-V_h^j(y))}{2} [Z_j^h; \varrho]_+ &= \frac{(V_h^j(x)-V_h^j(y))}{2} \mathbb{H}_{j,+}^h \widehat{\varrho} \\ \frac{(V_h^j(x)+V_h^j(y))}{2} [Z_j^h; \varrho]_- &= \frac{(V_h^j(x)+V_h^j(y))}{2} \mathbb{H}_{j,-}^h \widehat{\varrho} \end{aligned} \tag{120}$$

and by Wigner transform

$$\begin{aligned} \frac{1}{2} \Theta_- (V_h^j) \mathbb{H}_{j,+}^h \widehat{w} \\ \frac{1}{2} \Theta_+ (V_h^j) \mathbb{H}_{j,-}^h \widehat{w} \end{aligned} \tag{121}$$

for $h = 1, 2$ and $j = 1, 2, 3$.

From (120) and (121) it follows

$$\begin{aligned} \frac{1}{2} [\Theta_- (V_h^j) \mathbb{H}_{j,+}^h \widehat{w} + \Theta_+ (V_h^j) \mathbb{H}_{j,-}^h \widehat{w}] &= \frac{1}{2} [(\Theta_- (V_h^j) - \Theta_+ (V_h^j)) \mathbb{Z}_{j,1}^h] \widehat{w} + \\ &+ \frac{1}{2} [(\Theta_- (V_h^j) + \Theta_+ (V_h^j)) \mathbb{Z}_{j,2}^h] \widehat{w} \\ &= - \sum_{k=0}^{+\infty} \sum_{|\alpha|=k} (-i\hbar)^k \frac{\nabla^\alpha V_h^j(r)}{\alpha!} \mathbb{Z}_{j,1}^h \nabla^\alpha \widehat{w} + \\ &+ \sum_{k=0}^{+\infty} \sum_{|\alpha|=k} (i\hbar)^k \frac{\nabla^\alpha V_h^j(r)}{\alpha!} \mathbb{Z}_{j,2}^h \nabla^\alpha \widehat{w} \end{aligned} \tag{122}$$

By (122) we can write

$$\begin{aligned} \langle \mathcal{P}^{\otimes n} \mathcal{V} \widehat{w} \rangle &= \sum_{k=0}^{+\infty} \sum_{|\alpha|=k} (-i\hbar)^k \frac{\nabla^\alpha V_h^j}{\alpha!} \langle \mathcal{P}^{\otimes n} \mathbb{Z}_{j,1}^h \nabla^\alpha \widehat{w} \rangle + \\ &+ \sum_{k=0}^{+\infty} \sum_{|\alpha|=k} (i\hbar)^k \frac{\nabla^\alpha V_h^j}{\alpha!} \langle \mathcal{P}^{\otimes n} \mathbb{Z}_{j,2}^h \nabla^\alpha \widehat{w} \rangle \end{aligned} \tag{123}$$

where $\mathcal{P}^{\otimes n} = (p\widehat{1} - \frac{K}{2}\widehat{W}_-)^{\otimes n}$.

If we consider a single component $(p\widehat{1} - \frac{K}{2}\widehat{W}_-)^{\beta}$ of the tensor product $\mathcal{P}^{\otimes n}$, integration by parts yields

$$\left\langle \left(p\widehat{1} - \frac{K}{2}\widehat{W}_- \right)^{\beta} \mathbb{Z}_{j,v}^h \nabla^\alpha \widehat{w} \right\rangle = \begin{cases} (-1)^{|\alpha|} \left\langle \left(p\widehat{1} - \frac{K}{2}\widehat{W}_- \right)^{\beta-\alpha} \mathbb{Z}_{j,v}^h \widehat{w} \right\rangle & \text{if } \alpha \leq \beta \\ 0 & \text{if } \alpha \not\leq \beta \end{cases} \tag{124}$$

then

$$\langle \mathcal{P}^{\otimes n} \mathbb{Z}_{j,v}^h \nabla^\alpha \widehat{w} \rangle = (-1)^{|\alpha|} \langle \mathcal{P}^{\otimes(n-\alpha)} \mathbb{Z}_{j,v}^h \widehat{w} \rangle. \tag{125}$$

Let $\mathcal{P}^\gamma = (p\widehat{1} - \frac{K}{2}\widehat{W}_-)^{\gamma}$, with $|\gamma| = n - k$, be any component of $\mathcal{P}^{\otimes(n-\alpha)}$; then we can write

$$\begin{aligned} \left(p\widehat{1} - \frac{K}{2}\widehat{W}_- \right)^{\gamma} &= \sum_{\delta \leq \gamma} \binom{\gamma}{\delta} (p\widehat{1})^{\delta} \left(-\frac{K}{2}\widehat{W}_- \right)^{\gamma-\delta} \\ &= \sum_{\delta \leq \gamma} \binom{\gamma}{\delta} p^{\delta} \left(-\frac{K}{2} \right)^{\gamma-\delta} (\widehat{W}_-)^{|\gamma-\delta|} \end{aligned} \tag{126}$$

and

$$\begin{aligned} \left(p\widehat{1} - \frac{K}{2}\widehat{W}_- \right)^{\gamma} \mathbb{Z}_{j,v}^h &= \sum_{\delta \leq \gamma} \binom{\gamma}{\delta} p^{\delta} \left(-\frac{K}{2} \right)^{\gamma-\delta} (\widehat{W}_-)^{|\gamma-\delta|} \mathbb{Z}_{j,v}^h \\ &= \sum_{\delta \leq \gamma} \binom{\gamma}{\delta} \left(-\frac{K}{2} \right)^{\gamma-\delta} (\widehat{W}_-)^{|\gamma-\delta|} \mathbb{Z}_{j,v}^h p^{\delta} \\ &= \sum_{\delta \leq \gamma} \binom{\gamma}{\delta} \left(-\frac{K}{2} \right)^{\gamma-\delta} (\widehat{W}_-)^{|\gamma-\delta|} \mathbb{Z}_{j,v}^h \left(\mathcal{P} + \frac{K}{2}\widehat{W}_- \right)^{\delta}, \end{aligned} \tag{127}$$

since $\mathcal{P}\widehat{W}_- = \widehat{W}_-\mathcal{P}$, we obtain

$$\begin{aligned} \left(p\mathbb{1} - \frac{k}{2}\widehat{W}_-\right)^\gamma \mathbb{Z}_{j,v}^h &= \sum_{\eta \leq \delta \leq \gamma} \binom{\gamma}{\delta} \binom{\delta}{\eta} \left(-\frac{k}{2}\right)^{\gamma-\delta} \left(\widehat{W}_-\right)^{|\gamma-\delta|} \mathbb{Z}_{j,v}^h \left(\frac{k}{2}\widehat{W}_-\right)^{\delta-\eta} \mathcal{P}^\eta \\ &= \sum_{\eta \leq \delta \leq \gamma} \binom{\gamma}{\delta} \binom{\delta}{\eta} \left(-\frac{k}{2}\right)^{\gamma-\delta} \left(\widehat{W}_-\right)^{|\gamma-\delta|} \mathbb{Z}_{j,v}^h \left(\widehat{W}_-\right)^{|\delta-\eta|} \left(\frac{k}{2}\right)^{\delta-\eta} \mathcal{P}^\eta \end{aligned} \tag{128}$$

This shows that each component of $\langle \mathcal{P}^{\otimes(n-\alpha)} \mathbb{Z}_{j,v}^h \widehat{w} \rangle$ is a linear combination of terms $\langle \mathcal{P}^\gamma \widehat{w} \rangle$, with $|\gamma| \leq n - k$. In conclusion we get

$$\langle \mathcal{P}^{\otimes n} \mathcal{V} \widehat{w} \rangle = \sum_{k=0}^n \sum_{|\alpha|=k} \left(\frac{i\hbar}{2}\right)^k \frac{\nabla^\alpha V_h^j}{\alpha!} \langle \mathcal{P}^{\otimes(n-\alpha)} \mathbb{H}_{j,k}^h \widehat{w} \rangle \tag{129}$$

where $\mathbb{H}_{j,k}^h = \mathbb{Z}_{j,1}^h + (-1)^k \mathbb{Z}_{j,2}^h$ and $\langle \mathcal{P}^{\otimes(n-\alpha)} \mathbb{H}_{j,k}^h \widehat{w} \rangle$ is a linear combination of components of $\langle \mathcal{P}^\gamma \widehat{w} \rangle$, with $|\gamma| \leq n - |\alpha|$.

5. Two-band Madelung Equations

Proposition (2) and corollary (2) imply that the $n = 0$ and $n = 1$ moment equations for a pure state are closed and yield an analogue of QHD Madelung equations.

For $n = 0$, we get

$$\langle \mathcal{V} \widehat{w} \rangle = V_h^j(r) \mathbb{H}_{j,0}^h \langle \widehat{w} \rangle \tag{130}$$

where $\mathbb{H}_{j,0}^h = \mathbb{Z}_{j,1}^h + \mathbb{Z}_{j,2}^h$.

For $n = 1$ and $k = 0$, we have

$$V_h^j(r) \langle \mathcal{P} \mathbb{H}_{j,0}^h \widehat{w} \rangle = V_h^j(r) \mathbb{H}_{j,0}^h \langle \mathcal{P} \widehat{w} \rangle + V_h^j(r) [\widehat{W}_-; \mathbb{H}_{j,0}^h] \langle \widehat{w} \rangle. \tag{131}$$

For $n = 1$ and $k = 1$, we get

$$\left(\frac{i\hbar}{2}\right) \nabla V_h^j(r) \langle \mathbb{H}_{j,1}^h \widehat{w} \rangle = \left(\frac{i\hbar}{2}\right) \nabla V_h^j(r) \mathbb{H}_{j,1}^h \langle \widehat{w} \rangle \tag{132}$$

where $\mathbb{H}_{j,1}^h = \mathbb{Z}_{j,1}^h - \mathbb{Z}_{j,2}^h$; then

$$\langle \mathcal{P} \mathcal{V} \widehat{w} \rangle = V_h^j(r) \mathbb{H}_{j,0}^h J + V_h^j(r) [\widehat{W}_-; \mathbb{H}_{j,0}^h] n + \left(\frac{i\hbar}{2}\right) \nabla V_h^j(r) \mathbb{H}_{j,1}^h n. \tag{133}$$

Using (92), (130) and (5.4) we can write the moment equations for $n = 0$ and $n = 1$ in the following form

$$\begin{cases} \partial_t n + \frac{1}{m} \mathcal{D} J - \frac{ik^2}{2m\hbar} n = V_h^j(r) \mathbb{H}_{j,0}^h n \\ \partial_t J + \frac{1}{m} \mathcal{D} \left(\frac{J \otimes J}{n} + Q(n) - V(n)\right) - \frac{ik^2}{2m\hbar} J = V_h^j(r) \mathbb{H}_{j,0}^h J + [V_h^j(r) [\widehat{W}_-; \mathbb{H}_{j,0}^h] + \frac{i\hbar}{2} \nabla V_h^j(r) \mathbb{H}_{j,1}^h] n \end{cases} \tag{134}$$

5.1 The $\mathbb{Z}_{j,v}^h$ Matrices

$$\begin{aligned} \mathbb{Z}_{1,1}^1 &= \begin{pmatrix} \sigma_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \sigma_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sigma_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \sigma_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} & \mathbb{Z}_{1,2}^1 &= \begin{pmatrix} 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 \\ \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \\ \\ \mathbb{Z}_{1,1}^2 &= \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \sigma_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sigma_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \sigma_1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma_1 \end{pmatrix} & \mathbb{Z}_{1,2}^2 &= \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} \\ 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 \end{pmatrix} \end{aligned}$$

$$\begin{aligned} \mathbb{Z}_{2,1}^1 &= \begin{pmatrix} \sigma_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \sigma_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sigma_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \sigma_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} & \mathbb{Z}_{2,2}^1 &= \begin{pmatrix} 0 & 0 & -i\mathbf{1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i\mathbf{1} & 0 & 0 & 0 & 0 \\ i\mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & i\mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \\ \\ \mathbb{Z}_{2,1}^2 &= \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \sigma_2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sigma_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \sigma_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma_2 \end{pmatrix} & \mathbb{Z}_{2,2}^2 &= \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -i\mathbf{1} \\ 0 & 0 & 0 & 0 & 0 & 0 & -i\mathbf{1} & 0 \\ 0 & 0 & 0 & 0 & i\mathbf{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & i\mathbf{1} & 0 & 0 \end{pmatrix} \\ \\ \mathbb{Z}_{3,1}^1 &= \begin{pmatrix} a_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & b_3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sigma_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \sigma_3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} & \mathbb{Z}_{3,2}^1 &= \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\mathbf{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \\ \\ \mathbb{Z}_{1,1}^2 &= \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \sigma_3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sigma_3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & a_3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & b_3 \end{pmatrix} & \mathbb{Z}_{3,2}^2 &= \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\mathbf{1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \end{aligned}$$

with

$$a_3 = \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix}, \quad b_3 = \begin{pmatrix} 0 & 0 \\ 0 & -2 \end{pmatrix}.$$

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