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GENERAL AND APPLIED PHYSICS

An Introduction to Quantum Plasmas

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Abstract Shielding effects in non-degenerate and degenerate plasmas are compared. A detailed derivation of the Wigner-Poisson system is provided for electrostatic quantum plasmas in which relativistic, spin, and collisional effects are not essential. A detailed derivation of a quantum hydrodynamic model starting from the Wigner-Poisson system is presented. The route for this derivation considers the eikonal decomposition of the one-body wavefunctions of the quantum statistical mixture. The merits and limitations of the resulting quantum hydrodynamic model are discussed.

Keywords Quantum plasmas · Fermion systems · Electron gas · Quantum transport · Plasma kinetic equations

1 Introduction

Plasma physics is frequently not a part of the standard physics curriculum. Thus, theoretical physicists who study quantum mechanics are not usually exposed to plasma science and have no interest in it. And vice versa, plasma physicists often do not have the required background in quantum theory.

Plasma physics is commonly thought of as a purely classical field. Nonetheless, the last ten years have witnessed renewed interest in plasma systems marked by quantum effects; see [1–4] for extensive reviews. Quantum mechanics becomes relevant in plasmas when the de Broglie wavelength of the charge carriers is comparable to the inter-particle distance, so that there is a significant overlap of the corresponding wavefunctions. In such a situation, the many-body problem is described by Fermi-Dirac statistics, in contrast to the usual laboratory and space plasmas, which obey Maxwell-Boltzmann statistics. The fermionic character becomes prominent for sufficiently dense plasmas. Among these, one can cite plasmas in such compact astrophysical objects as white dwarfs and the atmosphere of neutron stars [5], or in the next generation intense-laser–solid-density plasma interaction experiments [6].

Moreover, many-body charged particle systems cannot be treated by pure classical physics when the characteristic dimensions become comparable to the de Broglie wavelength. This is the case for quantum semiconductor devices, like high-electron-mobility transistors, resonant tunneling diodes, or superlattices. The operation of these ultra-small devices relies on quantum tunneling of charge carriers through potential barriers. For these systems both Maxwell-Boltzmann or Fermi-Dirac statistics can be applied, according to the particle density. For instance, the Fermi-Dirac character should be taken into account in the drain region of n^+nn^+ diodes [7, 8]. In addition, due to recent advances in femtosecond pump-probe spectroscopy, quantum plasma effects are attracting attention in the physics of metallic nanostructures and thin metal films [9]. Also, X-ray Thomson scattering in high energy density plasmas provide experimental techniques for accessing narrow bandwidth spectral lines [10], so as to detect frequency shifts due to quantum effects. Such modifications of the plasmon dispersion relation are inline with theoretical predictions [11]. In this context,

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precise experiments have been suggested [12] in order to measure low-frequency collective oscillations (ion-acoustic waves) in dense plasmas, as soon as keV free electron lasers become available.

The purpose of this short introduction is two-fold. First, we present an elementary discussion on the screening of a test charge in non-degenerate and degenerate plasmas. Shielding is one of the most emblematic collective effects in plasmas, so that it is appropriate to comment on the differences between its classical and quantum regimes. In this way, a convenient introduction to quantum plasmas is provided. Second, we consider the basic kinetic and fluid models for quantum plasmas. We hence present the Wigner-Poisson system, which is the quantum equivalent of the Vlasov-Poisson system in classical plasma physics. Next, we discuss the derivation of fluid equations from the Wigner-Poisson model. Special attention is paid to the transition from microscopic to macroscopic descriptions. While none of these subjects is new, most of the calculations here are intended to be shown in more detail than the usual discussion in the literature. In an attempt to restrict the treatment to a basic level, only electrostatic, weakly coupled and non-relativistic quantum plasmas are considered. Hence, spin, magnetic field, collisional or relativistic effects are not addressed.

This work is organized as follows. In order to introduce the basic physical parameters for non-degenerate and degenerate plasmas, Section 2 discusses screening in these systems. Section 3 introduces the basic kinetic model for electrostatic quantum plasmas, namely the Wigner-Poisson system. Some of the fundamental properties of the Wigner function are analyzed, the Wigner function playing the rôle of a (quasi)-probability distribution in phase space. Section 4 applies an eikonal, or Madelung decomposition of the one-body wavefunctions defining the quantum statistical ensemble. In this way the pressure functional is shown to be the sum of two terms, associated with the kinetic and osmotic velocity dispersions (to be defined later), plus a Bohm potential term associated to quantum diffraction effects. Section 5 is dedicated to final remarks.

2 Shielding in Non-degenerate and Degenerate Plasmas

Suppose a test charge $q_t > 0$ is added to a plasma composed by an electron gas [of number density $n(\mathbf{r})$] and a fixed homogeneous ionic background (of number density n_0). Initially, due to the Coulomb force, the electron trajectories would deviate toward the test charge. Eventually, in the equilibrium situation, a stationary cloud of negative charge would accumulate around q_t. Then, instead of q_t an external observer would see an effective, smaller shielded charge. This is the (static) screening, or shielding effect in plasmas, in itself a manifestation of the quasi-neutrality property: due to the electric force, any excess charge tends to be compensated. In the stationary regime, the electrostatic field $\phi = \phi(\mathbf{r})$ is described by Poisson's equation,

$$\nabla^2\phi = \frac{e}{\varepsilon_0}\left(n(\mathbf{r}) - n_0\right) - \frac{q_t}{\varepsilon_0}\,\delta(\mathbf{r})\,, \tag{1}$$

where $-e < 0$ is the electron charge, ε_0 is vacuum permittivity, and for definiteness the test charge is located at the origin. For simplicity we assume the test charge to be sufficiently massive that it can be considered at rest.

Assuming a Maxwell-Boltzmann statistics, the quiescent electron gas being in thermodynamical equilibrium at a temperature T, one would have

$$n(\mathbf{r}) = n_0 \exp\left(\frac{e\phi}{\kappa_B T}\right)\,, \tag{2}$$

where κ_B is Boltzmann's constant.

The Maxwell-Boltzmann statistics is appropriate for dilute, or non-degenerate plasmas, for which the degeneracy parameter $\chi = T_F/T \ll 1$. Here $T_F = E_F/\kappa_B$ is the Fermi temperature, defined in terms of the Fermi energy [13]

$$E_F = \frac{\hbar^2}{2m}(3\pi^2 n_0)^{2/3}, \tag{3}$$

where $\hbar$ is Planck's constant over 2π and m is the electron mass. Since electrons are (spin-1/2) fermions, even in the limit of zero thermodynamic temperature it is impossible to accommodate all of them in the ground state, due to the Pauli exclusion principle. Hence, excited single-particle states are filled up until the highest energy level, whose corresponding energy is defined as E_F.

Assuming the scalar potential to be zero before the insertion of the test charge, we can linearize (1) to obtain

$$\nabla^2\phi = \frac{n_0 e^2}{\varepsilon_0 \kappa_B T}\,\phi - \frac{q_t}{\varepsilon_0}\,\delta(\mathbf{r})\,. \tag{4}$$

The radially symmetric solution to (4) with appropriate boundary conditions is the Yukawa potential

$$\phi = \frac{q_t}{4\pi\varepsilon_0 r}\,e^{-r/\lambda_D}\,, \tag{5}$$

where

$$\lambda_D = \left(\frac{\varepsilon_0 \kappa_B T}{n_0 e^2}\right)^{1/2} \tag{6}$$

is the (electron) Debye length. From (5), an observer would measure a very small potential for distances larger than the Debye length, which is inline with the linearization procedure. Therefore λ_D is a fundamental length for dilute, non-degenerate plasmas, playing the rôle of an effective range of the Coulomb interaction. Screening is a collective effect due to a large number of electrons around q_t.

What happens in the degenerate case? To start answering, notice that the number density (2) follows from the zeroth-order moment of the local Maxwell-Boltzmann one-particle equilibrium distribution function $f_{\rm cl} = f_{\rm cl}(\mathbf{r}, \mathbf{v})$ given by

$$f_{\rm cl}(\mathbf{r}, \mathbf{v}) = n_0 \left(\frac{m}{2\pi\kappa_B T}\right)^{3/2} \exp\left[-\frac{1}{\kappa_B T}\left(\frac{mv^2}{2} - e\phi\right)\right]. \tag{7}$$

In other words,

$$n(\mathbf{r}) = \int \mathrm{d}\mathbf{v}\, f_{\rm cl}(\mathbf{r}, \mathbf{v})\,. \tag{8}$$

On the other hand, the simplest approach for a degenerate plasma would consider an uniform distribution of electrons for energy smaller than the Fermi energy, and no particles above the Fermi level. Then (7) could be replaced by

$$f_{\rm cl}(\mathbf{r}, \mathbf{v}) = \begin{cases} \dfrac{3n_0}{4\pi v_F^3} & \text{if} \quad \dfrac{mv^2}{2} - e\phi < E_F, \\ 0 & \text{otherwise.} \end{cases} \tag{9}$$

In (9), $v_F = (2E_F/m)^{1/2}$ is the Fermi velocity. Notice the energy shift due to a nonzero scalar potential, the same shift defining the local Maxwell-Boltzmann equilibrium in (7). The distribution (9) is representative of a zero-temperature Thomas-Fermi equilibrium [14], displaying equal occupation probabilities for energies smaller than Fermi's energy, and no particles beyond. At this point, thermal effects are disregarded.

Equation (8) can be used to find the number density for the Thomas-Fermi equilibrium (9), yielding

$$n(\mathbf{r}) = n_0 \left(1 + \frac{e\phi}{E_F}\right)^{3/2}. \tag{10}$$

Inserting this result into Poisson's (1) and linearizing we get

$$\nabla^2\phi = \frac{3n_0e^2}{2\varepsilon_0 E_F}\,\phi - \frac{q_t}{\varepsilon_0}\,\delta(\mathbf{r}), \tag{11}$$

which is the same as (4) with the replacement $\kappa_B T \to E_F$, except for a numerical factor. Therefore, a shielding distance λ_F, or Thomas-Fermi length [3], can be set for degenerate plasmas,

$$\lambda_F = \left(\frac{2\varepsilon_0 E_F}{3n_0e^2}\right)^{1/2}. \tag{12}$$

Unlike the Debye length λ_D, the Thomas-Fermi length is nonzero even at zero thermodynamic temperature. This is due to the exclusion principle, which prevents the accumulation of electrons at the position occupied by the test charge.

Notice that in a sense every particle in a plasma, be it degenerate or not, can be interpreted as a test charge with the corresponding screening cloud. Hence instead of the long-range Coulomb field we have an effective Yukawa interaction field. This point of view is adopted, for instance, in the treatment of the ultrafast phase-space dynamics of ultracold, neutral plasmas [15].

In our simplified picture $f_{\rm cl}(\mathbf{r}, \mathbf{v})$ was regarded as a purely classical probability distribution function. A more detailed treatment taking into account quantum diffraction effects shows that at large distance the inter-particle oscillation behaves as

$$\phi \sim \frac{1}{r^3}\cos(2r/\lambda_F)\,, \tag{13}$$

a phenomenon known as *Friedel oscillations* [16, 17]. As discussed in the next Section, the Wigner function provides a convenient tool to incorporate quantum effects in plasmas, in strict analogy with the classical probability distribution approach.

The analysis of shielding introduces the characteristic length scales λ_D and λ_F in non-degenerate and degenerate plasmas, respectively. In addition, a length scale measuring the spatial extension of the wavefunction of each electron can be defined: the de Broglie wavelength $\lambda_B = \hbar/(mv_T)$, where $v_T = (2\kappa_B T/m)^{1/2}$ is the thermal velocity. Given the de Broglie wavelength one can express the degeneracy parameter as

$$\chi = \frac{T_F}{T} = \frac{1}{2}\left(3\pi^2 n_0 \lambda_B^3\right)^{2/3}. \tag{14}$$

Fermi-Dirac statistics becomes necessary when λ_B is of the order of the inter-particle distance.

Other fundamental scales in classical and quantum plasmas are as follows.

- Time scale for both classical and quantum plasmas: ω_p^{-1}, where

$$\omega_p = \left(\frac{n_0e^2}{m\varepsilon_0}\right)^{1/2}. \tag{15}$$

  is the plasma frequency. Given some electron charge depletion, an electric force appears in order

to restore complete charge neutrality. The resulting linear oscillations have frequency ω_p.

- Typical interaction energy $U_{\rm int}$ for both classical and quantum plasmas:

$$U_{\rm int} = \frac{e^2 n_0^{1/3}}{\varepsilon_0}\,, \tag{16}$$

since the mean inter-particle distance scales as $n_0^{-1/3}$.

- Typical kinetic energies: $K_C = \kappa_B T$ for non-degenerate and $K_Q = \kappa_B T_F$ for degenerate plasmas. The large fermionic kinetic energies are due to the Pauli exclusion principle, which forces excited states to be filled even at zero temperature.

From the typical energy scales we can form classical Γ_C and quantum Γ_Q energy coupling parameters,

$$\Gamma_C = \frac{U_{\rm int}}{K_C} = \frac{e^2 n_0^{1/3}}{\varepsilon_0 \kappa_B T} = 2.1 \times 10^{-4}\, \frac{n_0^{1/3}}{T}\,, \tag{17}$$

$$\Gamma_Q = \frac{U_{\rm int}}{K_Q} = \frac{2me^2}{(3\pi^2)^{2/3}\varepsilon_0 \hbar^2 n_0^{1/3}} = 5.0 \times 10^{10}\, n_0^{-1/3}\,. \tag{18}$$

The numerical values were calculated for S.I. units. Weakly coupled plasmas have small energy coupling parameters. From (17–18) the conclusion is that while classical weakly-coupled plasmas tend to be dilute and cold, quantum weakly-coupled plasmas tend to be dense. For example, with $n_0 > 10^{35} m^{-3}$ (white dwarf) one has $\Gamma_Q < 0.1$, allowing the use of collisionless models in a first approximation. This is a consequence of the Pauli exclusion principle, which tends to bar e-e collisions in very dense systems. In other words, the more dense a degenerate plasma is, the more it resembles an ideal gas, except for the mean field, collective interaction.

A more detailed account on the characteristic scales in classical and quantum Coulomb systems can be found in [1, 4, 18].

3 Obtaining the Wigner-Poisson System

The Vlasov-Poisson system

$$\frac{\partial f_{cl}}{\partial t} + v\frac{\partial f_{cl}}{\partial x} + \frac{e}{m}\frac{\partial \phi}{\partial x}\frac{\partial f_{cl}}{\partial v} = 0, \tag{19}$$

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{e}{\varepsilon_0}\left(\int {\rm d}v f_{cl}(x, v, t) - n_0\right) \tag{20}$$

is the basic tool in the kinetic theory of classical plasmas, where for simplicity we have considered a one-dimensional electron plasma in a fixed neutralizing ionic background n_0. In the Vlasov Eq. (19), $f_{cl} = f_{cl}(x, v, t)$ is the reduced one-particle probability distribution function. For a plasma with N electrons, $(1/N)\, f_{cl}(x, v, t)\, dv\, dx$ gives the probability of finding one electron with position between x and $x + dx$ and velocity between v and $v + dv$, at the time t. The normalization

$$\int {\rm d}v\, {\rm d}x\, f_{cl}(x, v, t) = N \tag{21}$$

is hence assumed.

Once the Vlasov-Poisson system subject to appropriate boundary conditions is solved, either analytically or numerically, to determine f_{cl}, the whole machinery of classical statistical mechanics becomes available to compute the expectation values of macroscopic quantities. For example, the average kinetic energy of one electron follows from

$$< \frac{mv^2}{2} >= \frac{1}{N}\int {\rm d}v\, {\rm d}x\, f_{cl}(x, v, t)\frac{mv^2}{2}. \tag{22}$$

It is convenient to adopt a similar methodology in a quantum kinetic theory for plasmas, as far as possible.

The Wigner function $f = f(x, v, t)$, a quantum equivalent of $f_{cl}(x, v, t)$, affords a phase-space formulation of quantum mechanics. Let us study some of its basic properties. For an one-particle pure state quantum system with wavefunction $\psi(x, t)$, the Wigner function is defined as [19]

$$f = \frac{m}{2\pi\hbar}\int ds\, \exp\left(\frac{i\, m\, v\, s}{\hbar}\right) \psi^*\left(x + \frac{s}{2}, t\right) \psi\left(x - \frac{s}{2}, t\right)\,, \tag{23}$$

with all symbols as before. From $f(x, v, t)$ we can compute the probability density

$$\int dv\, f(x, v, t) = |\psi(x, t)|^2 \tag{24}$$

and the probability current

$$\int dv\, f(x, v, t)\, v = \frac{i\hbar}{2m}\left(\psi\frac{\partial \psi^*}{\partial x} - \psi^*\frac{\partial \psi}{\partial x}\right)\,. \tag{25}$$

The wavefunction $\psi(x)$ is normalized to unity.

In general, even a one-particle quantum system cannot be represented by a single wavefunction. Mixed quantum states are described by a quantum statistical ensemble $\{\psi_\alpha(x, t)\,, p_\alpha\}$, $\alpha = 1, 2, ...M$, with each wavefunction $\psi_\alpha(x, t)$ having an occupation probability p_α

such that $p_\alpha \geq 0$, with $\sum_{\alpha=1}^{M} p_\alpha = 1$. The Wigner function is then defined by the superposition

$$f = \frac{m}{2\pi\hbar}\sum_{\alpha=1}^{M} p_\alpha \int ds \exp\left(\frac{i m v s}{\hbar}\right) \times \psi_\alpha^*\left(x+\frac{s}{2},t\right)\psi_\alpha\left(x-\frac{s}{2},t\right). \quad (26)$$

Correspondingly, we have the probability and current densities

$$\int dv\, f(x,v,t) = \sum_{\alpha=1}^{M} p_\alpha |\psi_\alpha(x,t)|^2, \quad (27)$$

$$\int dv\, f(x,v,t)\, v = \frac{i\hbar}{2m}\sum_{\alpha=1}^{M} p_\alpha\left(\psi_\alpha\frac{\partial\psi_\alpha^*}{\partial x} - \psi_\alpha^*\frac{\partial\psi_\alpha}{\partial x}\right). \quad (28)$$

The density matrix $\rho(x, y, t)$ could also be elected as the central object in a quantum kinetic theory for plasmas, but in this approach the similarity to the Vlasov-Poisson model would be lost. Besides, the formulation defined by (26–28) is in complete correspondence to the density-matrix formalism, since

$$\rho(x,y,t) \equiv \sum_{\alpha=1}^{M} p_\alpha\,\psi_\alpha(x,t)\,\psi_\alpha^*(y,t) = \int dv \exp\left(\frac{i m v (x-y)}{\hbar}\right) f\left(\frac{x+y}{2},v,t\right), \quad (29)$$

with inverse given by

$$f(x,v,t) = \frac{m}{2\pi\hbar}\int ds \exp\left(\frac{i m v s}{\hbar}\right)\rho\left(x+\frac{s}{2},x-\frac{s}{2},t\right). \quad (30)$$

In other words, given the Wigner function the density matrix can be found and vice-versa. The same applies to many-body Wigner functions and density matrices.

To proceed one step further, consider now a N-particle statistical mixture described by the set $\{\psi_\alpha^N(x_1, x_2, ..., x_N, t), p_\alpha\}$, where the normalized N-particle ensemble wavefunctions $\psi_\alpha^N(x_1, x_2, ..., x_N, t)$ are distributed with probabilities p_α, $\alpha = 1, 2, ..., M$ satisfying $p_\alpha \geq 0$, $\sum_{\alpha=1}^{M} p_\alpha = 1$ as before. Here x_i represents the position of the ith-particle, $i = 1, 2, ...N$. All particles have the same mass m. The N-particle Wigner function is defined by

$$f^N(x_1, v_1.., x_N, v_N, t) = N\left(\frac{m}{2\pi\hbar}\right)^N \sum_{\alpha=1}^{M} p_\alpha \int ds_1...ds_N \exp\left(\frac{i m \sum_{i=1}^{N} v_i s_i}{\hbar}\right) \times \psi_\alpha^{N*}\left(x_1+\frac{s_1}{2},...,x_N+\frac{s_N}{2},t\right) \times \psi_\alpha^{N}\left(x_1-\frac{s_1}{2},...,x_N-\frac{s_N}{2},t\right). \quad (31)$$

The factor N in (31) is inserted so that

$$\int dx_1 dv_1...dx_N dv_N\, f^N(x_1, v_1, ..., x_N, v_N, t) = N. \quad (32)$$

In this manner, the integral of f^N over all the velocities gives a number density in configuration space. The fermionic character of the system is not necessarily included, but this can be done by assuming the N-body ensemble wavefunctions to be antisymmetric in (31).

Wigner functions provide a convenient mathematical tool to calculate average quantities, and hence are analogous to the classical probability distribution function. Nonetheless, they are not necessarily positive definite. Hence it is customary to refer to them as quasi-probability distributions.

To proceed to the derivation of the quantum analog of the Vlasov-Poisson system (19) and (20), we can introduce the reduced one-particle Wigner function $f(x_1, v_1, t)$,

$$f(x_1, v_1, t) = \int dx_2 dv_2...dx_N dv_N\, f^N(x_1, v_1, ..., x_N, v_N, t), \quad (33)$$

and the reduced two-particle Wigner function $f^{(2)}(x_1, v_1, x_2, v_2, t)$, with a convenient normalization factor N,

$$f^{(2)}(x_1, v_1, x_2, v_2, t) = N\int dx_3 dv_3...dx_N dv_N\, f^N \times (x_1, v_1, ..., x_N, v_N, t). \quad (34)$$

Similar reduced N-particle Wigner functions with $N \geq 3$ can be likewise be defined. If the Wigner function were a true probability distribution, $(1/N)$ $f(x_1, v_1, t)dx_1dv_1$ would give the probability of finding the particle 1 in an area dx_1dv_1 centered at (x_1, v_1), irrespective of the "position" and "velocity" of the remaining ith-particles, $i = 2, ..., N$. An analogous

"classical" probability interpretation could be assigned to the remaining reduced Wigner functions, except for the non-positive-definiteness property.

In passing, we notice that

$$\int dx_1 dv_1 \, f(x_1, v_1, t) = N,$$

$$\int dx_1 dv_1 dx_2 dv_2 \, f^{(2)}(x_1, v_1, x_2, v_2, t) = N^2 . \tag{35}$$

It is reasonable to pay special attention to the reduced Wigner functions, since f^N contain far more information than what is commonly needed. In this regard the one-particle Wigner function plays a distinguished rôle. Indeed, macroscopic objects like number and current densities can be derived from f after integration over just one velocity variable, exactly as in (27) and (28), originally written for a one-particle system.

To obtain the evolution equation satisfied by the one-body Wigner function, the philosophy of [20] can be pursued. Consider then the Schrödinger equation satisfied by the N-body ensemble wavefunctions,

$$i\hbar \frac{\partial \psi_\alpha^N}{\partial t} = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \frac{\partial^2 \psi_\alpha^N}{\partial x_i^2} + V(x_1, ..., x_N)\, \psi_\alpha^N \tag{36}$$

for an interaction energy $V(x_1, ..., x_N)$.

We are concerned with cases in which the system components interact through some two-body potential W,

$$V(x_1, ..., x_N) = \sum_{i<j} W(|x_i - x_j|). \tag{37}$$

As it is evident, (37) is particularly interesting because it describes the Coulomb interaction.

Some algebra then shows that [1, 20]

$$\frac{\partial f}{\partial t} + v_1 \frac{\partial f}{\partial x_1} = -\frac{im}{2\pi\hbar^2} \int ds_1 \, dv_1' \, dx_2 \, dv_2' \times \exp\left(-\frac{im\,(v_1' - v_1)\, s_1}{\hbar}\right) \times \left(W\left(\left|x_1 - x_2 + \frac{s_1}{2}\right|\right) - W\left(\left|x_1 - x_2 - \frac{s_1}{2}\right|\right)\right) \times f^{(2)}(x_1, v_1', x_2, v_2', t), \tag{38}$$

which relates the reduced one-particle Wigner function f to the reduced two-particle Wigner function $f^{(2)}$. In the derivation, it was taken into account that $N \gg 1$. As a matter of fact, a more detailed argument involving the higher-order Wigner functions yield a quantum Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy [21–24], which shows the dynamics of the $(N-1)$-body reduced Wigner function to depend on the N-body reduced Wigner function. Hence in both the classical infinite BBGKY set of equations and its quantum analogue we are faced with a closure problem.

Ignoring correlations is the simplest way to close the system, i.e., assuming that the distribution of particles at (x_i, v_i) is unaffected by the particles at a distinct phase space point (x_j, v_j). In this mean field (or Hartree) approximation the N-body Wigner function factorizes,

$$f^{(2)}(x_1, v_1, x_2, v_2, t) = f(x_1, v_1, t)\, f(x_2, v_2, t). \tag{39}$$

Equation (38) then becomes

$$\frac{\partial f}{\partial t} + v_1 \frac{\partial f}{\partial x_1} = \int dv_1' \, K[W_{sc} \,|\, v_1' - v_1, x_1, t]\, f(x_1, v_1', t), \tag{40}$$

with the mean field self-consistent potential

$$W_{sc}(x, t) = \int dv \, dx' \, f(x', v, t)\, W(|x - x'|). \tag{41}$$

The functional $K[W_{sc} \,|\, v_1' - v_1, x_1, t]$ is defined by

$$K[W_{sc} \,|\, v_1' - v_1, x_1, t] = -\frac{im}{2\pi\hbar^2} \int ds_1 \, \exp\left(-\frac{im(v_1' - v_1)s_1}{\hbar}\right) \times \left(W_{sc}\left(x_1 + \frac{s_1}{2}, t\right) - W_{sc}\left(x_1 - \frac{s_1}{2}, t\right)\right). \tag{42}$$

Frequently an external, possibly time-dependent potential $V_{ext}(x_1, ..., x_N, t)$ should be included. Such a circumstance arises, for instance, in solid-state devices, when the electronic motion in a fixed ionic lattice or under a confining field like in quantum wires or quantum wells is considered [7, 8, 25]. Or even the field due to a homogeneous ionic background can be regarded as an external superimposed field. Hence, consider an external potential of the form

$$V_{ext}(x_1, ..., x_N, t) = \sum_{i=1}^{N} W_{ext}(x_i, t) \tag{43}$$

for some one-particle potential $W_{ext}(x_i, t)$. It is implicit in (43) that the functional form of W_{ext} is the same irrespective of x_i, so that the external field has the same influence on all particles. For completeness we record here the potential

$$V(x_1, ..., x_N) = \sum_{i<j} W(|x_i - x_j|) + \sum_{i=1}^{N} W_{ext}(x_i, t). \tag{44}$$

Following the same steps as before, the one-body reduced Wigner function $f(x_1, v_1, t)$ can then be shown to satisfy the equation

$$\frac{\partial f}{\partial t} + v_1 \frac{\partial f}{\partial x_1} = \int dv_1' K[W_{sc} + W_{ext} \mid v_1' - v_1, x_1, t] f(x_1, v_1', t), \quad (45)$$

for

$$K[W_{sc} + W_{ext} \mid v_1' - v_1, x_1, t] = -\frac{im}{2\pi\hbar^2} \int ds_1 \exp\left(-\frac{im(v_1' - v_1)s_1}{\hbar}\right) \times \left(W_{sc}\left(x_1 + \frac{s_1}{2}, t\right) + W_{ext}\left(x_1 + \frac{s_1}{2}, t\right) - W_{sc}\left(x_1 - \frac{s_1}{2}, t\right) - W_{ext}\left(x_1 - \frac{s_1}{2}, t\right)\right) \quad (46)$$

where the averaged self-consistent potential W_{sc} is again given by (41).

The necessary changes in three-dimensional charged particle motion are as follows. Consider, for definiteness, the Coulomb interaction

$$W(|\mathbf{r} - \mathbf{r}'|) = \frac{e^2}{4\pi\varepsilon_0 |\mathbf{r} - \mathbf{r}'|}. \quad (47)$$

and define the total electrostatic potential $\phi(\mathbf{r}, t)$ so that

$$\phi(\mathbf{r}, t) = \phi_{sc}(\mathbf{r}, t) + \phi_{ext}(\mathbf{r}, t), \quad (48)$$

the two terms on the right-hand side being associated with the self-consistent potential W_{sc} and some external potential W_{ext}. Explicitly,

$$W_{sc}(\mathbf{r}, t) = -e\phi_{sc}(\mathbf{r}, t), \quad \text{and} \quad W_{ext}(\mathbf{r}, t) = -e\phi_{ext}(\mathbf{r}, t). \quad (49)$$

From the three-dimensional version of (41) it follows that

$$\nabla^2\phi_{sc} = -\frac{e}{\varepsilon_0} \int d\mathbf{v}\, d\mathbf{r}'\, f(\mathbf{r}', \mathbf{v}, t)\, \nabla^2\left(\frac{1}{4\pi\,|\mathbf{r} - \mathbf{r}'|}\right) = \frac{e}{\varepsilon_0} \int d\mathbf{v}\, d\mathbf{r}'\, f(\mathbf{r}', \mathbf{v}, t)\, \delta(\mathbf{r} - \mathbf{r}') = \frac{e}{\varepsilon_0} \int d\mathbf{v}\, f(\mathbf{r}, \mathbf{v}, t). \quad (50)$$

Moreover,

$$\nabla^2\phi_{ext} = -\frac{1}{e}\nabla^2 W_{ext} \equiv -\frac{n_0 e}{\varepsilon_0} \quad (51)$$

if the external potential is due to an immobile fixed homogeneous ionic background of density n_0 and ion charge e. Appropriate changes are needed to describe a non-homogeneous background [7, 8, 25], e.g., in the case of doped semiconductors, or in the presence of a dispersive medium with permittivity constant $\varepsilon \neq \varepsilon_0$.

From (50) and (51) it is straightforward to derive the equality

$$\nabla^2\phi = \frac{e}{\varepsilon_0}\left(\int d\mathbf{v}\, f(\mathbf{r}, \mathbf{v}, t) - n_0\right), \quad (52)$$

the Poisson equation pertinent to the case under study.

Notational simplicity recommends that we once more restrict our discussion to the one-dimensional case. In terms of the electrostatic potential ϕ, (45) is rephrased as

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = \int dv'\, K_\phi[\phi \mid v' - v, x, t]\, f(x, v', t), \quad (53)$$

where $K_\phi[\phi \mid v' - v, x, t]$ is the functional

$$K_\phi[\phi \mid v' - v, x, t] = \frac{iem}{\hbar} \int \frac{ds}{2\pi\hbar} \exp\left(\frac{im(v' - v)s}{\hbar}\right) \times \left(\phi\left(x + \frac{s}{2}, t\right) - \phi\left(x - \frac{s}{2}, t\right)\right). \quad (54)$$

Equation (53) can be termed the quantum Vlasov equation (in the electrostatic case), since it is the quantum analog of the Vlasov equation satisfied by the reduced one-particle probability distribution function. Finally, the quantum Vlasov equation should be coupled to Poisson's equation,

$$\frac{\partial^2\phi}{\partial x^2} = \frac{e}{\varepsilon_0}\left(\int dv\, f(x, v, t) - n_0\right). \quad (55)$$

Equations (53) and (55) constitute the Wigner-Poisson system, which is the fundamental kinetic model for electrostatic quantum plasmas. It self-consistently determines both the Wigner function, associated with the particle distribution in phase space, and the scalar potential, which in turn describe the forces on the particles.

The Wigner-Poisson system needs to be supplemented with suitable boundary and initial conditions. For plasmas, decaying or periodic boundary conditions are frequently employed. For nanodevices, the choice of boundary conditions is subtler due to the finite size of the system and the nonlocal character of the Wigner function. Indeed, to compute the integral defining the Wigner function we need to specify $f(x, v, 0)$ over the entire space, even when dealing with finite size systems [7, 8, 25].

It seems appropriate, at this point, to recapitulate the simplifications in the derivation of the Wigner-Poisson system. Above all, it is a mean field model, with the N-body ensemble Wigner function assumed to be factorisable, in order to achieve the simplest closure of the quantum BBGKY hierarchy. Hence the N-body

Schrödinger equation (or the Liouville-von Neumann equation for the N-body ensemble density matrix) is replaced by a system with fewer degrees of freedom. Indeed, for N electrons in three-dimensional space, we have $3N+1$ coordinates to define the wavefunction, $6N+1$ coordinates for the density matrix, and only $6+1=7$ independent variables for the reduced one-body Wigner function, time taken into account here. The mean field theory is, therefore, much less numerically demanding, since it requires discretization of a space with fewer dimensions. The price for the reduction is the neglect of collisions, besides—at least in the present formulation—spin and relativistic effects. And finally, no magnetic fields were included.

Since it is the analog of the Vlasov-Poisson, the Wigner-Poisson system becomes the natural tool in quantum kinetic theory for electrostatic plasmas. With some optimism, the methods traditionally applied to the Vlasov-Poisson system can be translated to Wigner-Poisson quantum plasmas. Nevertheless, other quantum kinetic treatments of charged particle systems are obviously important. For example, the density-functional [25] and Green's function [26, 27] approaches are popular tools for the modeling quantum transport in the condensed matter community. Moreover, alternative approaches can sometimes overcome the simplifications of the Wigner-Poisson model. For instance, Green's function techniques can be used to describe collisions associated to short range particle-particle interactions [26, 27], in terms of a Boltzmann type collision operator.

It is instructive to examine the semiclassical limit of the quantum Vlasov (53). Combined with the change of variable $s=\hbar\tau/m$, a Taylor expansion leads to the approximate equality

$$\frac{\partial f}{\partial t}+v\frac{\partial f}{\partial x}+\frac{e}{m}\frac{\partial\phi}{\partial x}\frac{\partial f}{\partial v}=\frac{e\hbar^2}{24m^3}\frac{\partial^3\phi}{\partial x^3}\frac{\partial^3 f}{\partial v^3}+O(H^4). \tag{56}$$

Implicitly, the semiclassical approximation assumes the smallness of a non-dimensional quantum parameter $H=\hbar/(mv_0L_0)$, where v_0 and L_0 are characteristic velocity and length scales, respectively.

Equation (56) is a semiclassical Vlasov equation, with f playing the rôle of one-particle distribution function. We see that unlike the result for classical plasmas, in general neither f nor phase space volume are preserved by the quantum Vlasov equation, since

$$\frac{df}{dt}=\frac{e\hbar^2}{24m^3}\frac{\partial^3\phi}{\partial x^3}\frac{\partial^3 f}{\partial v^3}+O(H^4)\neq 0, \tag{57}$$

along the (classical) characteristic equations

$$\frac{dx}{dt}=v,\quad \frac{dv}{dt}=\frac{e}{m}\frac{\partial\phi}{\partial x}. \tag{58}$$

It follows that the positive definiteness of the Wigner function is not preserved by (53), except for linear electric field and vanishing quantum correction. Also notice that, although similar to, (57) is not truly a Boltzmann equation, since it remains invariant under time-reversal $t\to -t, x\to x, v\to -v$, $f(x,v,t)\to f(x,-v,-t)$ (assuming that $\phi(x,t)=\phi(x,-t)$). There is no irreversibility nor memory loss at all in the quantum Vlasov equation, be it in the semiclassical or the fully quantum versions. This is hardly surprising, since the Schrödinger equation is invariant under time reversal.

Even when the quantum Vlasov and Vlasov equations are the same, as in the case of linear electric fields, $f(x,v,t)$ cannot be viewed as an ordinary probability distribution function. Not all phase-space functions are acceptable as Wigner functions, since a genuine Wigner function corresponds necessarity to a positive definite density matrix. At least the following necessary conditions hence emerge [28],

$$\int dxdvf=N, \tag{59}$$

$$\int dvf\geq 0, \tag{60}$$

$$\int dxf\geq 0, \tag{61}$$

$$\int dxdvf^2\leq\frac{mN^2}{2\pi\hbar}. \tag{62}$$

Equation (59) is simply a normalization condition, while (60) and (61) assure the spatial and velocity marginal probability densities to be everywhere non-negative. Equation (62) eliminate excessively spiky Wigner functions, which would violate the uncertainty principle. For instance, for the Gaussian profile

$$f=\frac{N}{2\pi\sigma_x\sigma_v}\exp\left(-\frac{x^2}{2\sigma_x^2}\right)\exp\left(-\frac{v^2}{2\sigma_v^2}\right) \tag{63}$$

with constant standard deviations $\sigma_{x,v}$, it follows from (62) that

$$\sigma_x\sigma_v>\frac{\hbar}{2m}, \tag{64}$$

in accordance with the uncertainty principle.

Since no collisional effects are included in the Wigner-Poisson system, strongly coupled quantum plasmas require special treatment. Hence, in principle, the Wigner-Poisson model assumes a small energy

coupling parameter; see (17) and (18). For dense plasmas (such as the electron gas in metals), however, quantum collisionless models are sometimes still applicable thanks to the Pauli blocking of e-e collisions [4], even if the energy coupling parameter is large.

Not only very dense charged particle systems require quantum kinetic equations. For instance, due to the ongoing miniaturization, even scarcely populated electronic systems such as resonant tunneling diodes should be described by quantum models [7]. Indeed, the behavior of these ultra-small electronic devices relies on such quantum diffraction effects as tunneling, which makes purely classical methods inappropriate. The non-local integro-differential potential term in (53) in the Wigner-Poisson system has been shown to be able to model the negative differential resistance associated to tunneling [29]. Moreover, in view of the nanometric scale of the devices, the collisionless approximation becomes more reasonable, simply because the mean free-path exceeds the system size.

In the same manner, the usually extreme high operating frequencies makes the collisionless approximation more accurate, because $\omega\tau \ll 1$ for typical frequency ω and average time τ between collisions. For example, in resonant tunneling diodes potential barriers of the order $0.3\,eV \sim \hbar\omega$ are often found [7], which correspond to an operating frequency $\omega \sim 10^{15}\,s^{-1}$. The Wigner-Poisson system is therefore well suited for ballistic, collisionless processes in nanometric solid-state devices, even at relatively low densities $n_0 \sim 10^{24}m^{-3}$. The correspoinding Fermi temperature $T_F \sim 40K$, much smaller than the typical room temperature $T \sim 300K$, justifies the non-degeneracy assumption and Maxwell-Boltzmann's statistics.

4 Derivation of a Fluid Model for Quantum Plasmas

The Wigner-Poisson method presents some drawbacks: (a) it is a nonlocal, integro-differential system; (b) its numerical treatment requires the discretization of the entire phase space. Moreover, as is often the case with kinetic models, the Wigner-Poisson system gives more information than one is really interested in.

For these reasons, it would be useful to obtain an accurate reduced model which, though not providing the same detailed information as the kinetic Wigner-Poisson approach, might still be able to reproduce the main characteristics of quantum plasmas.

To obtain a set of macroscopic equations for quantum plasmas, we first derive a system of reduced 'fluid' equations by taking moments of the Wigner-Poisson system. Using a Madelung (or eikonal) decomposition, it can be shown that the pressure term appearing in the fluid equations can be separated into a classical and a quantum parts. A working hypothesis is then applied to the classical term, so as to close the fluid system. Shortly, the meaning of classical and quantum contributions to the pressure will be explained.

This approach to a quantum hydrodynamic model for plasmas appeared in [30]. The same quantum fluid model has been applied to several distinct problems involving charged particle systems, for instance, the nonlinear electron dynamics in thin metal films [9], the excitation of electrostatic wake fields in nanowires [31], parametric amplification characteristics in piezoelectric semiconductors [32], breather waves in semiconductor quantum wells [33], multidimensional dissipation-based Schrödinger models from quantum Fokker-Planck dynamics [34], the description of quantum diodes in degenerate plasmas [35] and quantum ion-acoustic waves in single-walled carbon nanotubes [36], to name but a few. The model was extended to incorporate magnetic fields in [37].

We take moments of (53) by integrating over the velocity space. In other words, introducing the standard definitions of density, mean velocity and pressure

$$n(x,t) = \int f\,dv, \quad u(x,t) = \frac{1}{n}\int fv\,dv,$$
$$P(x,t) = m\left(\int fv^2 dv - nu^2\right), \tag{65}$$

we get

$$\frac{\partial n}{\partial t} + \frac{\partial (nu)}{\partial x} = 0, \tag{66}$$
$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \frac{e}{m}\frac{\partial \phi}{\partial x} - \frac{1}{mn}\frac{\partial P}{\partial x}. \tag{67}$$

A more detailed theory would include the energy transport equation obtained after taking the second-order moment of the Wigner function and the associated time-derivative.

Equations (66) and (67) coincide with the ordinary evolution equations for a classical fluid. This may seem strange, but in the following it will be seen that the quantum nature of the system is in fact hidden in the pressure term. Contributions explicitly dependent on $\hbar$ are only found in the higher-order moments. For this reason, since in the electrostatic case $\hbar$ appears explicitly only in the equation of motion for the third-order moment [38], it is not enough to take only the energy transport equation into account.

To proceed, first notice the equivalence between the Wigner-Poisson and a system of countably many Schrödinger equations coupled to the Poisson equation, one that has been mathematically demonstrated [39].

More explicitily, the reduced one-body Wigner function can always be written as

$$f(x,v,t) = \frac{Nm}{2\pi\hbar}\sum_{\alpha=1}^{M} p_\alpha \int ds \times \exp\left(\frac{imvs}{\hbar}\right)\psi_\alpha^*\left(x+\frac{s}{2},t\right)\psi_\alpha\left(x-\frac{s}{2},t\right), \tag{68}$$

with an ensemble probability $p_\alpha \geq 0$, subject to the condition $\sum_{\alpha=1}^{M} p_\alpha = 1$, for each one-particle ensemble wavefunctions $\psi_\alpha(x,t)$ normalized to unity and satisfying

$$i\hbar\frac{\partial\psi_\alpha}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi_\alpha}{\partial x^2} - e\phi\psi_\alpha, \quad \alpha = 1,...,M, \tag{69}$$

which is the Schrödinger equation for a particle under the action of the mean field electrostatic potential $\phi(x,t)$. In addition, the Poisson (55) is rewritten as

$$\frac{\partial^2\phi}{\partial x^2} = \frac{e}{\varepsilon_0}\left(N\sum_{\alpha=1}^{M} p_\alpha|\psi_\alpha(x,t)|^2 - n_0\right). \tag{70}$$

Equations (69) and (70) constitute the so-called Schrödinger-Poisson system, which has to be supplemented with suitable initial and boundary conditions. It provides a way of replacing the original N-body problem by a collection of one-body Schrödinger equations, coupled by Poisson's equation. From a methodological point of view, the Schrödinger-Poisson modeling corresponds to putting the emphasis again on the wavefunction and not on the (phase-space) Wigner function. Collective effects are mediated by the self-consistent potential ϕ.

A rigorous proof of the equivalence between (69) and (70) and the Wigner-Poisson system [39] is beyond the scope of the present text. We can nonetheless gain some insight on the interpretation of the ensemble wavefunctions. From (31) and (33), we see that

$$\begin{aligned} f(x_1,v_1,t) &= \int dx_2dv_2...dx_Ndv_N\, f^N(x_1,v_1,...,x_N,v_N,t) \\ &= N\left(\frac{m}{2\pi\hbar}\right)\sum_{\alpha=1}^{M} p_\alpha \int ds_1\, dx_2...dx_N \\ &\quad\times\exp\left(\frac{imv_1s_1}{\hbar}\right)\psi_\alpha^{N*}\left(x_1+\frac{s_1}{2},x_2,...,x_N,t\right) \\ &\quad\times\psi_\alpha^N\left(x_1-\frac{s_1}{2},x_2,...,x_N,t\right). \end{aligned} \tag{71}$$

To be inline with the mean field approximation, it is natural to factorize the N-body wavefunction in the form

$$\psi_\alpha^N(x_1,x_2,...,x_N,t) = \psi_\alpha(x_1,t)\times...\times\psi_\alpha(x_N,t), \tag{72}$$

which fully neglects correlations. Quantum statistics effects are not taken into account in the *Ansatz* (72), which does not respect the Pauli principle. With this *caveat*, we insert (72) into (71), which yields precisely (68), with the same statistical weights p_α. Hence we can view the one-body ensemble wavefunctions $\psi_\alpha(x,t)$ as the result of splitting the N-body ensemble wavefunction into the product of identical factors. Of course, it is hardly surprising that a correlationless model can ultimately be written in terms of a collection of one-body Schrödinger equations.

Thanks to the Schrödinger-Poisson form, we are able to decompose the pressure term in a classical and a quantum part, as follows. Consider the Wigner distribution in (68). In terms of the ensemble wavefunctions, from (65) one obtains

$$n = N\sum_{\alpha=1}^{M} p_\alpha|\psi_\alpha|^2, \tag{73}$$

$$nu = \frac{i\hbar N}{2m}\sum_{\alpha=1}^{M} p_\alpha\left(\psi_\alpha\frac{\partial\psi_\alpha^*}{\partial x} - \psi_\alpha^*\frac{\partial\psi_\alpha}{\partial x}\right), \tag{74}$$

and, after some work,

$$P = \frac{N\hbar^2}{4m}\sum_{\alpha=1}^{M} p_\alpha\left(2\left|\frac{\partial\psi_\alpha}{\partial x}\right|^2 - \psi_\alpha^*\frac{\partial^2\psi_\alpha}{\partial x^2} - \psi_\alpha\frac{\partial^2\psi_\alpha^*}{\partial x^2}\right) + \frac{N^2\hbar^2}{4mn}\left[\sum_{\alpha=1}^{M} p_\alpha\left(\psi_\alpha^*\frac{\partial\psi_\alpha}{\partial x} - \psi_\alpha\frac{\partial\psi_\alpha^*}{\partial x}\right)\right]^2. \tag{75}$$

Now we follow Madelung [40] to decompose the wavefunctions in the form

$$\psi_\alpha(x,t) = A_\alpha(x,t)\exp\left(iS_\alpha(x,t)/\hbar\right), \tag{76}$$

where the amplitudes A_α and phases S_α are real functions. We then find the expressions

$$n = N\sum_{\alpha=1}^{M} p_\alpha A_\alpha^2, \tag{77}$$

$$nu = \frac{N}{m}\sum_{\alpha=1}^{M} p_\alpha A_\alpha^2\frac{\partial S_\alpha}{\partial x}, \tag{78}$$

and also

$$P = \frac{N^2}{2mn}\sum_{\alpha,\beta=1}^{M} p_\alpha p_\beta A_\alpha^2 A_\beta^2 \left(\frac{\partial S_\alpha}{\partial x} - \frac{\partial S_\beta}{\partial x}\right)^2 + \frac{N\hbar^2}{2m}\sum_{\alpha=1}^{M} p_\alpha \left[\left(\frac{\partial A_\alpha}{\partial x}\right)^2 - A_\alpha \frac{\partial^2 A_\alpha}{\partial x^2}\right]. \tag{79}$$

The constant $\hbar$ now appears explicitly on the right-hand side of the expression for the pressure. Notice, on the other hand, that since the ensemble wavefunctions satisfy the one-body Schrödinger (69) both the amplitudes and phases implicitly depend on Planck's constant.

It is useful to define the kinetic velocity u_α and the osmotic velocity u_α^o associated to the wavefunction ψ_α:

$$u_\alpha = \frac{1}{m}\frac{\partial S_\alpha}{\partial x}, \quad \text{and} \quad u_\alpha^o = \frac{\hbar}{m}\frac{\partial A_\alpha/\partial x}{A_\alpha}. \tag{80}$$

Then it can be verified that the pressure in (79) is given by

$$P = P^k + P^o + P^Q, \tag{81}$$

where the kinetic pressure P^k is

$$P^k = \frac{mn}{2}\sum_{\alpha,\beta=1}^{M} \tilde{p}_\alpha \tilde{p}_\beta (u_\alpha - u_\beta)^2, \tag{82}$$

the osmotic pressure P^o is

$$P^o = \frac{mn}{2}\sum_{\alpha,\beta=1}^{M} \tilde{p}_\alpha \tilde{p}_\beta (u_\alpha^o - u_\beta^o)^2, \tag{83}$$

and the quantum pressure P^Q is

$$P^Q = -\frac{\hbar^2 n}{4m}\frac{\partial^2}{\partial x^2}\ln n. \tag{84}$$

In (82) and (83), a modified set of ensemble probabilities $\tilde{p}_\alpha = \tilde{p}_\alpha(x,t)$ was introduced,

$$\tilde{p}_\alpha = \frac{N p_\alpha A_\alpha^2}{n}. \tag{85}$$

The new statistical weights satisfy $\tilde{p}_\alpha \geq 0$, $\sum_{\alpha=1}^{M} \tilde{p}_\alpha = 1$, as they should.

For a particular ψ_α the osmotic velocity points to the regions of higher density [41, 42], as is more evident in the three-dimensional version,

$$\mathbf{u}_\alpha^o = \frac{\hbar}{m}\nabla \ln A_\alpha. \tag{86}$$

Both pressures P^k and P^o can be viewed as a measure of the dispersion of the kinetic and osmotic velocities. Consider the following redefined average $< f_\alpha >$ of an ensemble function $f_\alpha = f_\alpha(x,t)$:

$$< f_\alpha >= \sum_{\alpha=1}^{M} \tilde{p}_\alpha f_\alpha. \tag{87}$$

Equations (82) and (83) are equivalent to the standard deviations

$$P^k = mn(\langle u_\alpha^2\rangle - \langle u_\alpha\rangle^2), \tag{88}$$

$$P^o = mn(\langle [u_\alpha^o]^2\rangle - \langle u_\alpha^o\rangle^2). \tag{89}$$

For a pure state so that $\tilde{p}_\alpha = \delta_{\alpha\beta}$ for some β, both P^k and P^o vanish, and only P^Q survives.

Since the kinetic and osmotic pressures measure the kinetic and osmotic velocity dispersions, it is reasonable, even if not rigorous, to assume an equation of state so that

$$P^k + P^o = P^C(n), \tag{90}$$

dependent only on the density. In this way, we obtain

$$P = P^C(n) - \frac{\hbar^2 n}{4m}\frac{\partial^2}{\partial x^2}\ln n. \tag{91}$$

For definiteness, we call P^C the "classical" part of the pressure, in the sense that it measures the dispersion of the velocities. However, it explicitly contains Planck's constant since it depends on the osmotic velocities, which always have a purely quantum nature.

The replacement of the sum of the kinetic and osmotic pressures by a function of the density requires only a few comments. Although exact, (81) offers no advantage over the Wigner-Poisson formulation, because it ultimately requires knowledge of the ensemble wavefunctions, and then the solution of a countable set of self-consistent Schrödinger equations. In classical kinetic theory (i.e., without the osmotic and quantum pressures), it is customary to reach closure by assuming that the standard deviation of the velocities is a function of the density only. We have gone just one step further, including also the standard deviation of the osmotic velocities.

In addition, in the classical limit we expect equations reproducing the classical fluid equations. This is certainly true if $P^k + P^o = P^C(n)$ for some appropriate function of density only. Finally, the standard Euler equations are reproduced thanks to the residual classical limit in P^k. Alternatively, for $\hbar \equiv 0$, we also have $P^o = 0$ and we expect P^k to be some function of the density only.

Unlike P in (65), which uses the Wigner function, the statistical weights in (88) and (89) are provided by the $\tilde{p}_\alpha$ in (85). For a pure state one has $P^C = 0$, which is inline with the understanding that a pure state

corresponds to a cold plasma with no dispersion of velocities. The contribution P^Q, on the other hand, finds no classical counterpart at all.

It has long been known that closure poses a delicate problem. The derivation of macroscopic models from microscopic models always call for some degree of approximation and a more or less phenomenological or ingenuous point of view. The present approach is capable of taking into account the quantum statistics of the charge carriers, represented by an appropriated equation of state. For example, assuming interaction with a heat bath an isothermal equation of state is indicated. For fast phenomena, in which thermal relaxation has no time to occur, an adiabatic equation of state can be used.

In the dilute or dense classes of plasmas, Maxwell-Boltzmann or Fermi-Dirac distributions can be employed, respectively. Moreover, the model accounts for quantum diffraction effects—in particular for tunneling and wave packet dispersion—, which are present in the quantum part P^Q of the pressure. It is also able to reproduce the linear dispersion relation from kinetic theory if the equation of state is adequate, except for purely kinetic phenomena. Finally, the quantum fluid model reduces to the standard Euler equations in the formal classical limit and are sufficiently simple to be amenable to efficient numerical simulation.

The proposed simplification becomes more justified for an important class of statistical ensembles, in which all the wavefunctions have equal amplitudes, although not necessarily constant ones,

$$\psi_\alpha = \sqrt{\frac{n}{N}}\, e^{iS_\alpha/\hbar}. \tag{92}$$

Then the osmotic pressure identically vanishes and one has $\tilde{p}_\alpha = p_\alpha$, so that (88) becomes the usual standard deviation of the kinetic velocities. Hence P^k can be interpreted in full analogy with the standard thermodynamic pressure. The velocity dispersion stems directly from the randomness of the phases of the wavefunctions. The approximation can be viewed as a first step beyond the standard homogeneous equilibrium of a fermion gas, for which each state can be represented by a plane wave

$$\psi_\alpha(x,t) = A_0 \exp\left(imu_\alpha x/\hbar\right), \tag{93}$$

with spatially constant amplitude A_0 and velocities u_α. In the generalization (92), both the amplitude and the velocity can be spatially modulated, although the amplitude is the same for all states. For systems not too far from equilibrium, this seems reasonable.

With the hypothesis (90), the force equation (67) can be written as

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = -\frac{1}{mn}\frac{\partial P^C(n)}{\partial x} + \frac{e}{m}\frac{\partial \phi}{\partial x} - \frac{1}{mn}\frac{\partial P^Q}{\partial x}. \tag{94}$$

Using the identity

$$\frac{1}{mn}\frac{\partial P^Q}{\partial x} = -\frac{\hbar^2}{2m^2}\frac{\partial}{\partial x}\left(\frac{\partial^2(\sqrt{n})/\partial x^2}{\sqrt{n}}\right), \tag{95}$$

we can rewrite the basic quantum hydrodynamic model for plasmas in terms of the continuity (66) and the force equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = -\frac{1}{mn}\frac{\partial P^C(n)}{\partial x} + \frac{e}{m}\frac{\partial \phi}{\partial x} + \frac{\hbar^2}{2m^2}\frac{\partial}{\partial x} \times \left(\frac{\partial^2(\sqrt{n})/\partial x^2}{\sqrt{n}}\right). \tag{96}$$

In the limit $\hbar \to 0$ this is formally equal to Euler's equation for an electron fluid in the presence of an electric field $-\partial\phi/\partial x$. Finally, we have the Poisson equation

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{e}{\varepsilon_0}(n - n_0), \tag{97}$$

The only difference from classical plasmas is the $\sim \hbar^2$ term in (96), the so-called Bohm potential term. While mathematically the Bohm potential is equivalent to a pressure to be inserted in the momentum transport equation, physically it corresponds to typical quantum phenomena like tunneling and wave packet spreading. Therefore it is not a pressure in the thermodynamic sense. Besides, it survives even for a one-particle pure-state system.

Many quantum hydrodynamical models are popular in the context of semiconductor physics. For instance, Gardner considered a quantum-corrected displaced Maxwellian distribution [43], as introduced by Wigner [19]. More exactly, it is possible to find the leading quantum correction $f_1(x,v,t)$ for a momentum-shifted local Maxwell-Boltzmann equilibrium $f_0(x,v,t)$, setting $f(x,v,t) = f_0(x,v,t) + \hbar^2 f_1(x,v,t)$ in the semi-classical quantum Vlasov (56) and collecting equal powers of $\hbar^2$. In other words set

$$f_0(x,v,t) = n(x,t)\left(\frac{m}{2\pi\kappa_B T(x,t)}\right)^{1/2} \times \exp\left(\frac{-m[v-u(x,t)]^2}{2\kappa_B T(x,t)}\right), \tag{98}$$

on the assumption of a non-degenerate quasi-equilibrium state. After calculating f_1, insert $f = f_0 + \hbar^2 f_1$ in the pressure in (65). A quantum hydrodynamical model similar to (66), (96), and (97) is then found (and generalized by the inclusion of

an energy transport equation). By definition, the resulting system is restricted to quasi-Maxwellian, dilute systems. We also observe that in the case of a self-consistent problem the electrostatic potential should have been also expanded in powers of some non-dimensional quantum parameter, which was not done in [43].

The conclusion is that the procedures involving a Madelung decomposition of the quantum ensemble wavefunctions or a quantum corrected Wigner function equilibrium involve working hypotheses which are not rigorously justified. Starting from the Wigner-Poisson system, which is by definition collisionless, and relying on quasi-equilibrium assumptions, one could hardly derive rigorous macroscopic theories. Nevertheless, the numerical and analytical advantages of quantum fluid models over quantum kinetic models make them much more popular than the kinetic treatment, to approach the nonlinear aspects of quantum plasma physics.

Alternatively, general thermodynamic arguments by Ancona and Tiersten have been used to derive the Bohm potential. Ancona and Tiersten [44] argues that the internal energy of the electron fluid in an electron-hole semiconductor should depend not only on the density, but also on the density gradient, in order to extend the standard drift-diffusion model so as to include the quantum-mechanical behavior in strong inversion layers. Their method defines a "double-force" and a "double-pressure vector" which allows for changes of the internal energy of the electron gas purely due to density fluctuations.

By postulating a linear dependence of the double-pressure vector on density gradients (see (3.3) of [44]) and working out the conservation laws of charge, mass, linear momentum and energy, Ancona and Tiersten found a generalized chemical potential comprising two contributions: (a) a gradient-independent term which can be modeled by the equation of state of a zero-temperature Fermi gas or any other appropriated form. This corresponds to the classical pressure $P^C(n)$ of the quantum hydrodynamical model for plasmas; (b) a Bohm potential term proportional to a phenomenological parameter initially left free.

Later, Ancona and Iafrate [45] obtained the expression of the phenomenological coefficient in [44]. In [45], which is similar to [43], the first order quantum correction for a Maxwell-Boltzmann equilibrium was found from the semiclassical quantum Vlasov equation and then employed to calculate the particle density and the stress tensor. The potential function eliminated between the two expressions, an equation of state relating the stress tensor and the particle density and gradient was derived, containing the Bohm potential.

The gradient dependence of the stress tensor is due to quantum mechanical nonlocality. Once again, the proof in [45] is valid when quantum contributions to the self-consistent mean field potential can be ignored: no expansion of ϕ in powers of a quantum parameter was used. Moreover, the plasma is assumed to be dilute and in the semiclassical regime, in which Maxwell-Boltzmann statistics is applicable and a small dimensionless quantum parameter exists.

Further, quantum hydrodynamic models with a "smoothed" potential have been derived, to handle discontinuities in potential barriers in semiconductors [46]. Energy transport [47] and quantum drift-diffusion [48] have been also employed to model transport in ultra-small electronic devices, including the addition of viscosity effects [49].

Quantum hydrodynamic models are well established in several specialties, even if the individual communities are unaware of the widespread dissemination. In molecular physics, for instance, the simplest gradient functional theory is given by the Thomas-Fermi-Dirac-von Weizsäcker functional, which provides a suitable expression for the energy density of molecules [50]. Its constituents are a Thomas-Fermi term for the uniform electron gas [51, 52], a Dirac exchange functional [53], the Coulomb term for the electron gas, a nuclear attraction term, and the von Weizsäcker term [54], with an adjustable fitting parameter. With this phenomenological parameter set to unity, the von Weissäcker term gives exactly the Bohm potential.

It is useful to remember the obvious limitations of the quantum hydrodynamic model for plasmas: (a) since it is a fluid model, it is applicable to long wavelengths only. This condition is expressed roughly as $\lambda > \lambda_D$ for non-degenerate and $\lambda > \lambda_F$ for degenerate systems, where λ is the pertinent wavelength. Kinetic phenomena, such as Landau damping or the plasma echo [55], call for detailed knowledge of the equilibrium Wigner function and hence require kinetic treatment; (b) no energy transport equation was included. This limitation, however, is not definitive, since it is a simple exercise to obtain the equation from the second-order moment of the quantum Vlasov equation; (c) it applies only to non-relativistic phenomena; (d) no spin effects are included, except for the equation of state which can, to a certain extent, represent some quantum statistical effects. It suffices to apply the equation of state for a dense, degenerate electron gas. In the same way, some relativistic effects can be also incorporated with an equation of state for a relativistic electron gas; (e) no magnetic fields are in the present formulation; (f) the sum of kinetic and osmotic pressures is assumed to be a function of the density only. This is in the spirit of

density-functional theories and appears reasonable in the vicinity of homogeneous equilibria, but may prove inappropriate far from equilibrium; (g) strongly coupled plasmas are out of reach since the starting point for the derivation was the quantum Vlasov equation, valid only for weak correlations.

It is remarkable that the eikonal decomposition method, starting from the Wigner-Maxwell system, allows inclusion of magnetic fields [37], the resulting quantum hydrodynamic model being modified simply by the addition of a magnetic $\sim \mathbf{u} \times \mathbf{B}$ force.

5 Concluding Remarks

Quantum plasma theory started in the 1950's with the analysis of the ground state and correlation energies of the dense electron gas in metals [56–58], with quantum field-theoretical techniques. Pioneering works [17, 20, 59] also focused on collective oscillation modes in dense plasmas, described by the collisionless quantum Boltzmann equation. Following a more or less quiescent period, in the last decade a new wave of interest in quantum plasmas was observed. Besides new applications to diverse systems ranging from nanoscale electronic devices and dense astrophysical environments to intense-laser–solid-density plasma interaction experiments, the emergence of efficient macroscopic models has attracted new attention to quantum plasmas. This short introduction has been essentially dedicated to the analysis of the transition from the microscopic (kinetic) to macroscopic (fluid) modeling of quantum plasmas.

Quantum plasma physics is a rapidly growing field, with unpredictable consequences. Below we list other fundamental topics currently under scrutiny, which for brevity were not not discussed here.

- The dynamics of spin degrees of freedom and the underlying ferromagnetic behavior in quantum plasmas [60–64].
- Relativistic quantum plasma models [65–68], an essential subject, since quantum and relativistic effects often appear simultaneously, e.g., in applications to compact astrophysical objects and intense laser plasmas.
- Extensions to include exchange-correlation and collisional contributions. The anti-symmetric nature of the N-body wavefunction introduces a Hartree-Fock term in the interaction energy [20]. However, such nonlocal exchange-correlation terms are frequently replaced by local phenomenological expressions, along with the adiabatic local-density approximation [69, 70]. Also, we mention the Wigner-Fokker-Planck system approach to model quantum dissipation [34, 71].

Last but not least, we mention that this introductory text was focused on the detailed *derivation* of the basic kinetic and hydrodynamic models for quantum plasmas, in a language meant to be accessible to beginners. A more complete account of the current *applications* of such quantum plasma models can be found in [1–4].

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