

Chapter 2

The Wigner–Poisson System

Abstract In electrostatic quantum plasmas, the Wigner–Poisson system plays the same rôle as the Vlasov–Poisson system in classical plasmas. This chapter considers the basic properties of the Wigner–Poisson system, including the essentials on the Wigner function method and the derivation of the Wigner–Poisson system in the context of a mean field theory. This chapter also contains a discussion on the Schrödinger–Poisson system as well as extensions to include correlation and collisional effects. The Wigner–Poisson system is shown to imply, in the high-frequency limit, the Bohm–Pines dispersion relation for linear waves, which is the quantum analog of the Bohm–Gross dispersion relation for classical plasmas.

2.1 The Wigner Function

To maintain the closest resemblance to the familiar methods of classical plasma physics, the Wigner function approach is the natural choice. Indeed, using the Wigner function, one can proceed in almost total analogy with the standard phase-space distribution function method to compute macroscopic quantities like number and current densities. Hence, it is useful to review some of the properties of the Wigner (pseudo) distribution function approach. In addition, the differences between classical and quantum formalisms will be highlighted. The treatment is by no means exhaustive, being intentionally restricted to the bare necessary minimum. More complete reviews on Wigner function methods can be found, for example, in [8, 18, 26, 36].

For simplicity, let us start with a one-dimensional, one-particle pure state quantum system, represented by a wavefunction $\psi(x, t)$. In this case, the Wigner function $f = f(x, v, t)$ is defined [38] as

$$f = \frac{m}{2\pi\hbar} \int ds \exp\left(\frac{imvs}{\hbar}\right) \psi^*\left(x + \frac{s}{2}, t\right) \psi\left(x - \frac{s}{2}, t\right), \quad (2.1)$$

where x is the position, v the velocity, t the time, m the particle's mass and $\hbar = h/(2\pi)$, where h is Planck's constant. In the above equation, the integration limits goes from minus to plus infinity, a convention followed except otherwise stated. The Wigner function provides a phase-space description of the quantum system where all physical quantities can be found from the k th-order moments $\int dv v^k f(x, v, t)$. For instance, both the probability density

$$n(x, t) = |\psi(x, t)|^2 = \int dv f(x, v, t) \quad (2.2)$$

and the probability current

$$J(x, t) = \frac{i\hbar}{2m} \left(\psi \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial \psi}{\partial x} \right) = \int dv v f(x, v, t) \quad (2.3)$$

can be readily obtained, respectively, from the zeroth and first order moments of the Wigner function. Here, we assume ψ normalized to unity. Moreover, the Wigner function is always real, differently from the wavefunction which is complex.

In the more general case of a mixed state, the one-dimensional, one-particle system is represented by a quantum statistical mixture $\{\psi_\alpha(x, t), p_\alpha\}$, $\alpha = 1, 2, \dots, M$, where each wavefunction $\psi_\alpha(x, t)$ occurs with a probability p_α such that $p_\alpha \geq 0$, $\sum_{\alpha=1}^M p_\alpha = 1$. In such a situation, the Wigner function is given by the superposition

$$f = \frac{m}{2\pi\hbar} \sum_{\alpha=1}^M p_\alpha \int ds \exp\left(\frac{imvs}{\hbar}\right) \psi_\alpha^*\left(x + \frac{s}{2}, t\right) \psi_\alpha\left(x - \frac{s}{2}, t\right). \quad (2.4)$$

The corresponding generalization of (2.2) and (2.3) is then

$$n(x, t) = \sum_{\alpha=1}^M p_\alpha |\psi_\alpha(x, t)|^2 = \int dv f(x, v, t), \quad (2.5)$$

$$J(x, t) = \frac{i\hbar}{2m} \sum_{\alpha=1}^M p_\alpha \left(\psi_\alpha \frac{\partial \psi_\alpha^*}{\partial x} - \psi_\alpha^* \frac{\partial \psi_\alpha}{\partial x} \right) = \int dv v f(x, v, t). \quad (2.6)$$

Notice that the quantum fluid probability $n(x, t)$ and the current density $J(x, t)$ are still given in terms of the zeroth- and first-order moments of $f(x, v, t)$.

The Wigner formalism can be rephrased in the density matrix $\rho(x, y, t)$ language, since

$$\rho(x, y, t) \equiv \sum_{\alpha=1}^M p_\alpha \psi_\alpha(x, t) \psi_\alpha^*(y, t) = \int dv \exp\left(\frac{imv(x-y)}{\hbar}\right) f\left(\frac{x+y}{2}, v, t\right), \quad (2.7)$$

with the inverse transformation being

$$f(x, v, t) = \frac{m}{2\pi\hbar} \int ds \exp\left(\frac{imvs}{\hbar}\right) \rho\left(x + \frac{s}{2}, x - \frac{s}{2}, t\right). \quad (2.8)$$

In the sense of the equivalence implied by (2.7) and (2.8), the use of the Wigner function or the density matrix is just a question of taste.

From the Wigner function, we can readily derive the marginal probability distributions in coordinate and momentum space. Indeed, from (2.8), it follows that

$$\int dv f = \rho(x, x, t) \quad (2.9)$$

and

$$\int dx f = m\tilde{\rho}(p, p', t), \quad (2.10)$$

where

$$\tilde{\rho}(p, p', t) = \frac{1}{2\pi\hbar} \int dx dx' \exp\left(\frac{i}{\hbar}(p'x' - px)\right) \rho(x, x', t) \quad (2.11)$$

denotes the matrix components of the density operator in the momentum representation, with $p = mv$, $p' = mv'$.

Going one step further, consider now a N -particle statistical mixture described by the set $\{\psi_\alpha^N(x_1, x_2, \dots, x_N, t), p_\alpha\}$, where the normalized N -particle ensemble wavefunctions $\psi_\alpha^N(x_1, x_2, \dots, x_N, t)$ are distributed with probabilities p_α , $\alpha = 1, 2, \dots, M$ satisfying $p_\alpha \geq 0$, $\sum_{\alpha=1}^M p_\alpha = 1$ as before. Here, x_i represents the position of the i th-particle, $i = 1, 2, \dots, N$. For simplicity, assume all particles to have the same mass m . In analogy with (2.4) the N -particle Wigner function is then defined as

$$\begin{aligned} f^N(x_1, v_1, \dots, x_N, v_N, t) &= N \left(\frac{m}{2\pi\hbar}\right)^N \sum_{\alpha=1}^M p_\alpha \int ds_1, \dots, ds_N \exp\left(\frac{im \sum_{i=1}^N v_i s_i}{\hbar}\right) \\ &\quad \times \psi_\alpha^{N*}\left(x_1 + \frac{s_1}{2}, \dots, x_N + \frac{s_N}{2}, t\right) \\ &\quad \times \psi_\alpha^N\left(x_1 - \frac{s_1}{2}, \dots, x_N - \frac{s_N}{2}, t\right). \end{aligned} \quad (2.12)$$

The factor N in (2.12) is inserted so that

$$\int dx_1 dv_1, \dots, dx_N dv_N f^N(x_1, v_1, \dots, x_N, v_N, t) = N. \quad (2.13)$$

In this manner, the integral of f^N over all the velocities gives a number density. For simplicity, at this stage we are not taking into account the usually fermionic character of the charged particles in plasma, so that the N -body ensemble wavefunctions are not necessarily antisymmetrized.

From the N -particle Wigner function, the expectation value of any observable can be computed in the same way as in classical statistical mechanics. In other words, $f(x_1, v_1, \dots, x_N, v_N, t)$ act as a weight in the same sense of the classical N -body particle distribution function $f_{\text{cl}}^N(x_1, v_1, \dots, x_N, v_N, t)$. In this context, we have that $(1/N) f_{\text{cl}}^N(x_1, v_1, \dots, x_N, v_N, t) dx_1 dv_1, \dots, dx_N dv_N$ gives the probability of the particle 1 being in an area $dx_1 dv_1$ in phase space centered at position x_1 and velocity v_1 , the particle 2 being in an area $dx_2 dv_2$ centered at position x_2 and velocity v_2 and so on. However, the Wigner function is not positive definite, so that it is not a probability but a pseudo-probability distribution.

More exactly, suppose a classical phase-space function $A(x_1, v_1, \dots, x_N, v_N, t)$ corresponding to a self-adjoint quantum mechanical operator $\hat{A}(\hat{x}_1, \hat{v}_1, \dots, \hat{x}_N, \hat{v}_N, t)$. Here, the hats denote operators and everything could be rewritten in terms of momenta and not velocities. We prefer to use velocities instead of momenta to assure a manifestly gauge invariant formalism. In addition, the transition from functions to operators is by no means unique: a well-defined correspondence rule should be employed [18, 26]. Special care should be paid with more complicated phase space observables involving noncommuting objects like products of functions of position and momenta. Indeed, to calculate expectation values using the Wigner formalism, we need first to map the observable into a phase-space function using the Weyl correspondence [37]. In practice, this is equivalent to ordering operators into a symmetric product of the position and momenta operators, using the commutation relations and then making the replacements $\hat{x}_i \rightarrow x_i$ and $\hat{p}_i \rightarrow p_i$, where \hat{x}_i, \hat{p}_i are the position and momentum operators of the i th-particle and x_i, p_i the corresponding classical position and momentum functions.

Given a classical function $A(x_1, v_1, \dots, x_N, v_N, t)$ the phase-space average $\langle A \rangle_{\text{cl}}$ is

$$\langle A \rangle_{\text{cl}} = \frac{1}{N} \int dx_1 dv_1, \dots, dx_N dv_N f_{\text{cl}}^N(x_1, v_1, \dots, x_N, v_N, t) A(x_1, v_1, \dots, x_N, v_N, t), \quad (2.14)$$

while the expectation value $\langle \hat{A} \rangle$ of the associated Weyl ordered self-adjoint operator $\hat{A}(\hat{x}_1, \hat{v}_1, \dots, \hat{x}_N, \hat{v}_N, t)$ is

$$\langle \hat{A} \rangle = \frac{1}{N} \int dx_1 dv_1, \dots, dx_N dv_N f^N(x_1, v_1, \dots, x_N, v_N, t) A(x_1, v_1, \dots, x_N, v_N, t). \quad (2.15)$$

We have an explicit resemblance between classical and quantum formalisms.

As an example, one can be interested in the expectation value of the total energy of an interacting system with potential energy $V(x_1, \dots, x_N)$. This average is given by

$$\frac{1}{N} \int dx_1 dv_1, \dots, dx_N dv_N f^N(x_1, v_1, \dots, x_N, v_N, t) \left(\sum_{i=1}^N \frac{mv_i^2}{2} + V(x_1, \dots, x_N) \right), \quad (2.16)$$

which is the same expression used in classical statistical mechanics, with the replacement $f_{\text{cl}}^N \rightarrow f^N$.

As already remarked, to obtain nonerroneous expectation values of operators involving noncommuting observables using the Wigner formalism, the Weyl ordering should be employed. To see an illustrative example, consider the operator

$$\begin{aligned}\hat{x}_i \hat{p}_j &= \frac{1}{2}(\hat{x}_i \hat{p}_j + \hat{p}_j \hat{x}_i) + \frac{1}{2}[\hat{x}_i, \hat{p}_j] \\ &= \frac{1}{2}(\hat{x}_i \hat{p}_j + \hat{p}_j \hat{x}_i) + \frac{i\hbar \delta_{ij}}{2} \\ &\rightarrow x_i p_j + \frac{i\hbar \delta_{ij}}{2} \quad (\text{Weyl rule}),\end{aligned}\tag{2.17}$$

using the commutation relation $[\hat{x}_i, \hat{p}_j] = i\hbar \delta_{ij}$ and where in the last equality the Weyl correspondence was applied. Hence, the required expectation value is

$$\langle \hat{x}_i \hat{p}_j \rangle = \frac{m}{N} \int dx_1 dv_1, \dots, dx_N dv_N f^N(x_1, v_1, \dots, x_N, v_N, t) x_i v_j + \frac{i\hbar \delta_{ij}}{2}, \tag{2.18}$$

taking into account $p_j = mv_j$. Indeed, after some integrations by parts the right-hand side of (2.18) is found to be

$$\begin{aligned}&\frac{m}{N} \int dx_1 dv_1, \dots, dx_N dv_N f^N(x_1, v_1, \dots, x_N, v_N, t) x_i v_j + \frac{i\hbar \delta_{ij}}{2} \\ &= -i\hbar \sum_{\alpha=1}^M p_\alpha \int dx_1, \dots, dx_N \psi_\alpha^{N*}(x_1, \dots, x_N, t) x_i \frac{\partial}{\partial x_j} \psi_\alpha^N(x_1, \dots, x_N, t),\end{aligned}\tag{2.19}$$

in line with the coordinate representation $\hat{p}_j \rightarrow -i\hbar \partial / \partial x_j$ of the momentum operator \hat{p}_j (not to confound with the ensemble probabilities p_α).

In addition to the Wigner function, alternative quantum probability distribution functions can be constructed. Among them, we can cite at least the Glauber–Sudarshan function [11, 34], the Q-function [12], the Husimi function [19], the Kirkwood distribution function [22] and the standard-ordered distribution function [32]. For these alternative functions, the underlying quantum-classical correspondence is given by specific methods other than the Weyl rule [8, 26]. The relevance of the non-Wigner probability distributions is recognized for specific purposes. For instance, the Q-functions and the Husimi functions can be shown to be everywhere nonnegative [26]. However, the Wigner function has a number of simultaneous attractive properties which makes it more popular than the other distribution functions. For example, the Q and Husimi functions does not provide the marginal probability distributions in coordinate and momentum space in the sense of (2.9) and (2.10), besides not satisfying certain closure properties [8, 26].

We note that in some places in the literature the Q-function and Husimi's function are considered as synonymous, as a brief survey reveal. However, although their expressions are the same, their correspondence rules are not, see [26].

2.2 Mean Field Approximation

In analogy to classical statistical mechanics, it is useful to introduce the reduced one-particle Wigner function $f(x_1, v_1, t)$,

$$f(x_1, v_1, t) = \int dx_2 dv_2, \dots, dx_N dv_N f^N(x_1, v_1, \dots, x_N, v_N, t), \quad (2.20)$$

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

$$f^{(2)}(x_1, v_1, x_2, v_2, t) = N \int dx_3 dv_3, \dots, dx_N dv_N f^N(x_1, v_1, \dots, x_N, v_N, t), \quad (2.21)$$

as well as the remaining reduced i -particle Wigner functions, $i = 3, \dots, N$. If the Wigner function were a true probability distribution, $(1/N) f(x_1, v_1, t) dx_1 dv_1$ would give the probability of finding the particle 1 in an area $dx_1 dv_1$ centered at (x_1, v_1) , irrespective of the “position” and “velocity” of the i th-particles, $i = 2, \dots, N$. The other partial, or reduced Wigner functions would have a similar interpretation.

What is the evolution equation satisfied by the N -body Wigner function? To answer the question, we follow the philosophy of [24]. Let us start from the Schrödinger equation satisfied by the N -body ensemble wavefunctions,

$$i\hbar \frac{\partial \psi_\alpha^N}{\partial t} = -\frac{\hbar^2}{2m} \sum_{i=1}^N \frac{\partial^2 \psi_\alpha^N}{\partial x_i^2} + V(x_1, \dots, x_N) \psi_\alpha^N \quad (2.22)$$

for a potential energy $V(x_1, \dots, x_N)$.

From (2.12) and (2.22),

$$\begin{aligned} \frac{\partial f^N}{\partial t} = & N \left(\frac{m}{2\pi\hbar} \right)^N \sum_{\alpha=1}^M p_\alpha \int ds_1, \dots, ds_N \exp \left(\frac{im \sum_{i=1}^N v_i s_i}{\hbar} \right) \\ & \times \left[\frac{i\hbar}{2m} \sum_{j=1}^N \left(\psi_\alpha^{N*}(\mathbf{x}_+, t) \frac{\partial^2 \psi_\alpha^N(\mathbf{x}_-, t)}{\partial x_j^2} - \frac{\partial^2 \psi_\alpha^{N*}(\mathbf{x}_+, t)}{\partial x_j^2} \psi_\alpha^N(\mathbf{x}_-, t) \right) \right. \\ & \left. + \frac{i}{\hbar} (V(\mathbf{x}_+) - V(\mathbf{x}_-)) \psi_\alpha^{N*}(\mathbf{x}_+, t) \psi_\alpha^N(\mathbf{x}_-, t) \right]. \end{aligned} \quad (2.23)$$

Above, we introduced the displaced collective coordinates

$$\mathbf{x}_+ = (x_1 + s_1/2, \dots, x_N + s_N/2), \quad (2.24)$$

$$\mathbf{x}_- = (x_1 - s_1/2, \dots, x_N - s_N/2). \quad (2.25)$$

To deal with (2.23) and similar equations, the following two identities are useful,

$$\begin{aligned} & \psi_{\alpha}^{N*}(\mathbf{x}_+, t) \frac{\partial^2 \psi_{\alpha}^N(\mathbf{x}_-, t)}{\partial x_i^2} - \frac{\partial^2 \psi_{\alpha}^{N*}(\mathbf{x}_+, t)}{\partial x_i^2} \psi_{\alpha}^N(\mathbf{x}_-, t) \\ &= -2 \frac{\partial^2}{\partial x_i \partial s_i} [\psi_{\alpha}^{N*}(\mathbf{x}_+, t) \psi_{\alpha}^N(\mathbf{x}_-, t)], \end{aligned} \quad (2.26)$$

$$\begin{aligned} & N \sum_{\alpha=1}^M p_{\alpha} \psi_{\alpha}^{N*}(\mathbf{x}_+, t) \psi_{\alpha}^N(\mathbf{x}_-, t) \\ &= \int d\mathbf{v}_1, \dots, d\mathbf{v}_N \exp\left(-\frac{im \sum_{i=1}^N v_i s_i}{\hbar}\right) f^N(x_1, v_1, \dots, x_N, v_N, t). \end{aligned} \quad (2.27)$$

From these identities and after integration by parts, (2.23) is converted into

$$\begin{aligned} & \frac{\partial f^N}{\partial t} + \sum_{i=1}^N v_i \frac{\partial f^N}{\partial x_i} \\ &= \int d\mathbf{v}'_1, \dots, d\mathbf{v}'_N \times K^N[V | v'_1 - v_1, x_1, \dots, v'_N - v_N, x_N, t] f^N(x_1, v'_1, \dots, x_N, v'_N, t), \end{aligned} \quad (2.28)$$

introducing the functional

$$\begin{aligned} & K^N[V | v'_1 - v_1, x_1, \dots, v'_N - v_N, x_N, t] \\ &= -\frac{i}{\hbar} \left(\frac{m}{2\pi\hbar}\right)^N \int d\mathbf{s}_1, \dots, d\mathbf{s}_N \exp\left(-\frac{im \sum_{i=1}^N (v'_i - v_i) s_i}{\hbar}\right) (V(\mathbf{x}_+) - V(\mathbf{x}_-)). \end{aligned} \quad (2.29)$$

In principle for a given interaction potential solving (2.28) amounts to a complete description of the N -body quantum problem. However, the development of analytic and numerical techniques for the N -body problem is of course a tremendous task. Moreover, for practical reasons, it is more effective to deal with the reduced Wigner functions, since f^N contain far more information than what is needed. In this regard, the one-particle Wigner function $f(x, v, t)$ plays a privileged rôle. Indeed, most macroscopic objects like number $n(x, t)$ and current $J(x, t)$ densities can be derived from the moments of $f(x, v, t)$,

$$n(x, t) = \int dv f(x, v, t), \quad (2.30)$$

$$J(x, t) = \int dv f(x, v, t) v, \quad (2.31)$$

much in the same way as in the classical formalism, in the transition from kinetic to fluid models. We also observe that (2.5) and (2.6) hold for a one-particle quantum fluid system, differently than (2.30) and (2.31) which apply to the N -body problem.

From the above reasoning, it is clearly relevant to obtain the evolution equation for the one-body reduced function $f(x, v, t)$. We are specially concerned with the case where the system components interact through some two-body potential W ,

$$V(x_1, \dots, x_N) = \sum_{i < j} W(|x_i - x_j|). \quad (2.32)$$

The importance of such a situation is evident due to the Coulomb forces present in charged particle systems.

Integrating (2.28) in the $(x_2, v_2, \dots, x_N, v_N)$ variables, it follows that

$$\begin{aligned} \frac{\partial f}{\partial t} + v_1 \frac{\partial f}{\partial x_1} &= -\frac{im}{2\pi\hbar^2} \int ds_1 dx_2 \dots dx_N dv'_1, \dots, dv'_N \exp\left(-\frac{im(v'_1 - v_1)s_1}{\hbar}\right) \\ &\quad \times \sum_{i=1}^N \left(W\left(|x_1 - x_i + \frac{s_1}{2}|\right) - W\left(|x_1 - x_i - \frac{s_1}{2}|\right) \right) \\ &\quad \times f^N(x_1, v'_1, \dots, x_N, v'_N, t). \end{aligned} \quad (2.33)$$

A change of variables shows that the latter can be written as

$$\begin{aligned} \frac{\partial f}{\partial t} + v_1 \frac{\partial f}{\partial x_1} &= -\frac{im}{2\pi\hbar^2} \int ds_1 dv'_1 dx_2 dv'_2 \exp\left(-\frac{im(v'_1 - v_1)s_1}{\hbar}\right) \\ &\quad \times \left(W\left(|x_1 - x_2 + \frac{s_1}{2}|\right) - W\left(|x_1 - x_2 - \frac{s_1}{2}|\right) \right) \\ &\quad \times f^{(2)}(x_1, v'_1, x_2, v'_2, t). \end{aligned} \quad (2.34)$$

in terms of the reduced two-particle Wigner function $f^{(2)}$ defined in (2.21). In the derivation $N \gg 1$ was taken into account. Actually, a more detailed argument involving the higher-order Wigner functions yield a quantum BBGKY (Bogoliubov–Born–Green–Kirkwood–Yvon) hierarchy [3, 6, 23, 39], where the dynamics of the $(N-1)$ -body reduced Wigner function is shown 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.

The simpler way to deal with the truncation problem is by ignoring correlations, assuming that the distribution of particles at (x_i, v_i) is not affected by particles at a distinct phase space point (x_j, v_j) . In this mean field (or Hartree) approximation, the N -body Wigner function factorizes so that in a first approximation

$$f^{(2)}(x_1, v_1, x_2, v_2, t) = f(x_1, v_1, t) f(x_2, v_2, t). \quad (2.35)$$

Now (2.34) simplifies to

$$\frac{\partial f}{\partial t} + v_1 \frac{\partial f}{\partial x_1} = \int dv'_1 K[W_{\text{sc}} | v'_1 - v_1, x_1, t] f(x_1, v'_1, t), \quad (2.36)$$

with the mean field explicitly time-dependent self-consistent potential

$$W_{\text{sc}}(x, t) = \int dx' dv f(x', v, t) W(|x - x'|). \quad (2.37)$$

The functional $K[W_{\text{sc}} | v'_1 - v_1, x_1, t]$ is given by

$$\begin{aligned} K[W_{\text{sc}} | v'_1 - v_1, x_1, t] = & -\frac{im}{2\pi\hbar^2} \int ds_1 \exp\left(-\frac{im(v'_1 - v_1)s_1}{\hbar}\right) \\ & \times \left(W_{\text{sc}}\left(x_1 + \frac{s_1}{2}, t\right) - W_{\text{sc}}\left(x_1 - \frac{s_1}{2}, t\right) \right). \end{aligned} \quad (2.38)$$

In many cases, it is necessary to take into consideration an external, possibly time-dependent potential $V_{\text{ext}}(x_1, \dots, x_N, t)$. For instance, such a circumstance arises in solid state devices, when considering the electronic motion in a fixed ionic lattice or under a confining field like in quantum wires or quantum wells [10, 20, 30]. Or even we can simply incorporate the field due to an homogeneous ionic background. In these cases, the external potential is of the form

$$V_{\text{ext}}(x_1, \dots, x_N, t) = \sum_{i=1}^N W_{\text{ext}}(x_i, t) \quad (2.39)$$

for some one-particle potential $W_{\text{ext}}(x_i, t)$. Implicitly in (2.39), the functional form of W_{ext} is the same irrespective of x_i , implying that the external field impose the same effect in all particles, which are supposed indistinguishable. Hence, for completeness, we indicate the changes for a potential

$$V(x_1, \dots, x_N) = \sum_{i < j} W(|x_i - x_j|) + \sum_{i=1}^N W_{\text{ext}}(x_i, t). \quad (2.40)$$

Repeating the steps in the derivation involving a self-consistent potential only, the time-evolution for the one-body reduced Wigner function $f(x_1, v_1, t)$ can then be shown to be governed by

$$\frac{\partial f}{\partial t} + v_1 \frac{\partial f}{\partial x_1} = \int dv'_1 K[W_{\text{sc}} + W_{\text{ext}} | v'_1 - v_1, x_1, t] f(x_1, v'_1, t), \quad (2.41)$$

where

$$\begin{aligned}
 K[W_{\text{sc}} + W_{\text{ext}} | v'_1 - v_1, x_1, t] &= -\frac{im}{2\pi\hbar^2} \int ds_1 \exp\left(-\frac{im(v'_1 - v_1)s_1}{\hbar}\right) \\
 &\quad \times \left(W_{\text{sc}}\left(x_1 + \frac{s_1}{2}, t\right) + W_{\text{ext}}\left(x_1 + \frac{s_1}{2}, t\right) \right. \\
 &\quad \left. - W_{\text{sc}}\left(x_1 - \frac{s_1}{2}, t\right) - W_{\text{ext}}\left(x_1 - \frac{s_1}{2}, t\right) \right) \quad (2.42)
 \end{aligned}$$

and the averaged self-consistent potential W_{sc} is as in (2.37).

2.3 Electrostatic Quantum Plasmas

Consider now three-dimensional charged particle motion, with the Coulomb interaction

$$W(|\mathbf{r} - \mathbf{r}'|) = \frac{e^2}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|}, \quad (2.43)$$

where $-e$ is the electron charge and ϵ_0 is the vacuum permittivity constant. In terms of the self-consistent W_{sc} and some external W_{ext} potentials, it is convenient to define the total electrostatic potential $\phi(\mathbf{r}, t)$ so that

$$\phi(\mathbf{r}, t) = \phi_{\text{sc}}(\mathbf{r}, t) + \phi_{\text{ext}}(\mathbf{r}, t), \quad (2.44)$$

where

$$W_{\text{sc}}(\mathbf{r}, t) = -e\phi_{\text{sc}}(\mathbf{r}, t), \quad W_{\text{ext}}(\mathbf{r}, t) = -e\phi_{\text{ext}}(\mathbf{r}, t). \quad (2.45)$$

It follows from the three-dimensional version of (2.37) that

$$\begin{aligned}
 \nabla^2 \phi_{\text{sc}} &= -\frac{e}{\epsilon_0} \int d\mathbf{r}' d\mathbf{v} f(\mathbf{r}', \mathbf{v}, t) \nabla^2 \left(\frac{1}{4\pi |\mathbf{r} - \mathbf{r}'|} \right) \\
 &= \frac{e}{\epsilon_0} \int d\mathbf{r}' d\mathbf{v} f(\mathbf{r}', \mathbf{v}, t) \delta(\mathbf{r} - \mathbf{r}') \\
 &= \frac{e}{\epsilon_0} \int d\mathbf{v} f(\mathbf{r}, \mathbf{v}, t). \quad (2.46)
 \end{aligned}$$

Moreover,

$$\nabla^2 \phi_{\text{ext}} = -\frac{1}{e} \nabla^2 W_{\text{ext}} \equiv -\frac{n_0 e}{\epsilon_0} \quad (2.47)$$

if the external potential is caused by an immobile fixed homogeneous ionic background of density n_0 and ion charge e . Appropriate changes are needed in the case of a nonhomogeneous background, for example, as in the case of doped semiconductors, or in presence of a dispersive medium with a permittivity constant $\epsilon \neq \epsilon_0$ [10, 20, 30].

Combining (2.46) and (2.47), it is immediate to obtain

$$\nabla^2 \phi = \frac{e}{\epsilon_0} \left(\int d\mathbf{v} f(\mathbf{r}, \mathbf{v}, t) - n_0 \right), \quad (2.48)$$

which is the Poisson equation in this case.

Just for notational simplicity, it is better to restrict again to the one-dimensional case. In this way the expressions look nicer, and the transition to three spatial dimensions can be easily done if necessary. In terms of the electrostatic potential ϕ , (2.41) is rephrased as

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} = \int dv' K_\phi[\phi | v' - v, x, t] f(x, v', t), \quad (2.49)$$

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

$$\begin{aligned} K_\phi[\phi | v' - v, x, t] &= \frac{iem}{\hbar} \int \frac{ds}{2\pi\hbar} \exp\left(\frac{im(v' - v)s}{\hbar}\right) \\ &\times \left(\phi\left(x + \frac{s}{2}, t\right) - \phi\left(x - \frac{s}{2}, t\right) \right). \end{aligned} \quad (2.50)$$

Equation (2.49) 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 distribution function. The quantum Vlasov equation for the Wigner function should be coupled to the Poisson equation for the scalar potential,

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{e}{\epsilon_0} \left(\int dv f(x, v, t) - n_0 \right). \quad (2.51)$$

Equations (2.49) and (2.51) constitute the Wigner–Poisson system, which is the fundamental model for electrostatic quantum plasmas. It determines in a self-consistent way both the Wigner function, associated with how the particles distribute in phase space, and the scalar potential, which in turn describe the forces acting on the particles.

Equations (2.49) and (2.51) need to be supplemented with suitable boundary and initial conditions. For plasmas, frequently decaying or periodic boundary conditions are sufficient. For nano-devices, 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 $f(x, v, 0)$ in the whole space even when dealing with finite size systems. We refer to the specialized literature for more details [10, 20, 30].

Before seeking some of the consequences of the Wigner–Poisson system, let us recapitulate the steps toward its derivation. First, it is a mean field model with the N -body ensemble Wigner function supposed to be factorisable. Thanks to this property, we achieved the simplest solution to the closure problem of the quantum

BBGKY hierarchy. In particular, it follows a notable advantage over the N -body Schrödinger equation (or equivalently over the Liouville–von Neumann equation for the N -body ensemble density matrix): the tremendous reduction of the number of independent variables. For $N \gg 1$ electrons in three-dimensional space, we can compare the $3N + 1$ coordinates entering the wavefunction, the $6N + 1$ coordinates of the density matrix, and the $6 + 1 = 7$ independent variables of the reduced one-body Wigner function, taking into account time. In particular, the mean field theory is much less numerically demanding, since it requires the discretization of a space with fewer dimensions. However, since correlations are disregarded, the Wigner–Poisson system does not incorporate collisions. Moreover, no spin or relativistic effects are taken into account in our presentation. Finally, no magnetic fields were introduced yet.

Once the Wigner–Poisson system has been derived, it becomes the natural tool in quantum kinetic theory for plasmas, since it is exactly analog to the Vlasov–Poisson system. Hence, the methods applied to the Vlasov–Poisson system can with some optimism be directly translated to quantum plasmas. Other quantum kinetic treatments for assemblies of charged particle systems are obviously important, but cannot compete with the Wigner formalism in the quantum plasma context. For instance, the density functional [10] and Green’s function [17, 21] approaches are popular tools for the modeling of quantum transport in the condensed matter community. However, presently the majority of the plasma physics researchers feels more comfortable with the particle distribution function method where the Vlasov equation plays a central rôle and for which a number of analytical and numerical methods are already available. Nevertheless, the simplifications underlying the Wigner–Poisson model points to the relevance of the alternative approaches toward a more sophisticated modeling. For instance, using Green’s function techniques to describe collisions associated with short range particle–particle interactions one finds [17, 21] a nonlocal Boltzmann type collision operator which has to be included in (2.49). However, these developments are outside the scope of the present text.

It is instructive to analyze the semiclassical limit of the quantum Vlasov equation (2.49). By means of the change of variable $s = \hbar \tau / m$ and Taylor expanding, the result is

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} - \frac{eE}{m} \frac{\partial f}{\partial v} = -\frac{e\hbar^2}{24m^3} \frac{\partial^2 E}{\partial x^2} \frac{\partial^3 f}{\partial v^3} + O(H^4), \quad (2.52)$$

where the electric field is $E = E(x, t) = -\partial\phi/\partial x$. Implicitly, the semiclassical approximation assumes the smallness of a nondimensional quantum parameter $H = \hbar/(mv_0 L_0)$, where v_0 and L_0 are, respectively, typical velocity and length scales.

If no quantum effects were present, (2.52) reduces to Vlasov’s equation,

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} - \frac{eE}{m} \frac{\partial f}{\partial v} = 0, \quad (2.53)$$

to be coupled to Poisson’s equation to compose the Vlasov–Poisson system.

As an intermediate step in the derivation of (2.52), one need to calculate integrals like

$$\begin{aligned} \int \frac{dv' d\tau}{2\pi} \tau e^{i(v'-v)\tau} f(x, v', t) &= i \frac{\partial}{\partial v} \int \frac{dv' d\tau}{2\pi} e^{i(v'-v)\tau} f(x, v', t) \\ &= i \frac{\partial}{\partial v} \int dv' \delta(v' - v) f(x, v', t) = i \frac{\partial f}{\partial v}. \end{aligned} \quad (2.54)$$

It is immediate to recognize (2.52) as a semiclassical Vlasov equation, with f playing the rôle of one-particle distribution function. From the Wigner function, one can compute macroscopic quantities like particle, current and energy densities, very much like in classical physics. Hence, it is a natural trend, to investigate to which extent the methods applied to the Vlasov–Poisson system can be useful in the Wigner–Poisson context. However, unlike in the classical limit, in general neither f nor phase space volume are preserved by the quantum Vlasov equation, since

$$\frac{df}{dt} = -\frac{e\hbar^2}{24m^3} \frac{\partial^2 E}{\partial x^2} \frac{\partial^3 f}{\partial v^3} + O(H^4) \neq 0 \quad (2.55)$$

along the (classical) characteristic equations $\dot{x} = v, \dot{v} = -eE/m$. Moreover the positive definiteness of the Wigner function is not preserved by (2.49). The exception is for linear electric fields, for which the quantum corrections vanishes in (2.52). In this case, the Wigner and Vlasov equations coincide to all orders in the nondimensional quantum parameter H .

Even in the harmonic oscillator case, when the Wigner and Vlasov equations coincide, $f(x, v, t)$ cannot be considered as an ordinary probability distribution function. Indeed, not all functions on phase space can be taken as Wigner functions, since a genuine Wigner function should correspond to a positive definite density matrix. Therefore, at least the following necessary conditions [18] must hold,

$$\int dx dv f = N, \quad (2.56)$$

$$\int dv f \geq 0, \quad (2.57)$$

$$\int dx f \geq 0, \quad (2.58)$$

$$\int dx dv f^2 \leq \frac{mN^2}{2\pi\hbar}. \quad (2.59)$$

Equation (2.56) is just a normalization condition, while (2.57) and (2.58) arise because the spatial and velocity marginal probability densities should be everywhere nonnegative. Finally, (2.59) is needed to avoid violation of the uncertainty principle, eliminating too spiky functions $f(x, v, t)$.

2.4 The Schrödinger–Poisson System

The equivalence between the Wigner–Poisson and a system of countably many Schrödinger equations coupled to the Poisson equation has been mathematically demonstrated [29]. More exactly, any Wigner function can be written as

$$f(x, v, t) = \frac{Nm}{2\pi\hbar} \sum_{\alpha=1}^M p_{\alpha} \int ds \exp\left(\frac{imvs}{\hbar}\right) \psi_{\alpha}^*\left(x + \frac{s}{2}, t\right) \psi_{\alpha}\left(x - \frac{s}{2}, t\right), \quad (2.60)$$

with ensemble probabilities $p_{\alpha} \geq 0$ so that $\sum_{\alpha=1}^M p_{\alpha} = 1$, for each one-particle ensemble wavefunctions $\psi_{\alpha}(x, t)$ satisfying

$$i\hbar \frac{\partial \psi_{\alpha}}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi_{\alpha}}{\partial x^2} - e\phi \psi_{\alpha}, \quad \alpha = 1, \dots, M, \quad (2.61)$$

which is the Schrödinger equation for a particle under the action of the mean field potential $\phi(x, t)$. In addition, the Poisson equation (2.51) is rewritten as

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{e}{\epsilon_0} \left(N \sum_{\alpha=1}^M p_{\alpha} |\psi_{\alpha}(x, t)|^2 - n_0 \right). \quad (2.62)$$

Equations (2.61) and (2.62) 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 problems, coupled by Poisson’s equation. From a methodological point of view, the Schrödinger–Poisson modeling corresponds to put 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 [29] of the equivalence of (2.61) and (2.62) and the Wigner–Poisson system (2.49)–(2.51) is beyond the present text. However, we can obtain some insight on the interpretation of the ensemble wavefunctions. From (2.12)–(2.20),

$$\begin{aligned} f(x_1, v_1, t) &= \int dx_2 dv_2, \dots, dx_N dv_N f^N(x_1, v_1, \dots, x_N, v_N, t) \\ &= N \left(\frac{m}{2\pi\hbar} \right) \sum_{\alpha=1}^M p_{\alpha} \int ds_1 dx_2, \dots, dx_N \exp\left(\frac{imv_1 s_1}{\hbar}\right) \\ &\quad \times \psi_{\alpha}^{N*}\left(x_1 + \frac{s_1}{2}, x_2, \dots, x_N, t\right) \psi_{\alpha}^N\left(x_1 - \frac{s_1}{2}, x_2, \dots, x_N, t\right). \end{aligned} \quad (2.63)$$

To follow the mean field approximation, we are tempted to assume the factorized form

$$\psi_{\alpha}^N(x_1, x_2, \dots, x_N, t) = \psi_{\alpha}(x_1, t) \times \dots \times \psi_{\alpha}(x_N, t), \quad (2.64)$$

for the N -body wavefunction, fully neglecting the correlations due to the interaction potential. Quantum statistics effects are not taken into account in the *Ansatz* (2.64), which does not respect the Pauli principle. However, for simplicity spin considerations will be not included at this moment. Inserting (2.64) into (2.63), the result is precisely (2.60), 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.

Equation (2.60) shows that the reduced one-body Wigner function is always in the form of the sum

$$f(x, v, t) = \sum_{\alpha=1}^M p_\alpha f_\alpha(x, v, t), \quad (2.65)$$

where

$$f_\alpha(x, v, t) = \frac{Nm}{2\pi\hbar} \int ds \exp\left(\frac{imvs}{\hbar}\right) \psi_\alpha^*\left(x + \frac{s}{2}, t\right) \psi_\alpha\left(x - \frac{s}{2}, t\right). \quad (2.66)$$

The case where only one ensemble wavefunction is needed so that $p_\alpha = \delta_{\alpha\beta}$ for some β corresponds to a pure state. Otherwise, we have a mixed state.

Using the map (2.7) from the Wigner function to the density matrix $\rho(x, y, t)$, we can derive a condition for a pure state. Supposing

$$f(x, v, t) = \frac{Nm}{2\pi\hbar} \int ds e^{\frac{imvs}{\hbar}} \psi^*\left(x + \frac{s}{2}, t\right) \psi\left(x - \frac{s}{2}, t\right) \quad (2.67)$$

in terms of a single wavefunction $\psi(x, t)$ and inserting in (2.7), we obtain

$$\rho(x, y, t) = N \psi(x, t) \psi^*(y, t). \quad (2.68)$$

Hence,

$$\frac{\partial^2 \ln \rho(x, y, t)}{\partial x \partial y} = 0 \quad (2.69)$$

is a necessary condition for a pure state, where $\rho(x, y, t)$ is given by (2.7). In addition to (2.69), a real Wigner function is required to qualify a pure state, which means $\rho^*(x, y, t) = \rho(y, x, t)$. Moreover, it can be shown that a pure state at $t = 0$ remains a pure state along the time-evolution of the quantum Vlasov equation (2.49).

While the direct construction using (2.60) of the Wigner function from the wavefunctions and the statistical weights is a trivial task, the reverse problem of how to choose ψ_α, p_α to reproduce a given Wigner function is more obscure. In particular, when we know we are dealing with a mixed state, what is the minimal number M of ensemble wavefunctions needed? Or, for a fixed M , what could be the natural way to define the wavefunctions ψ_α and the corresponding probabilities p_α so as to reproduce $f(x, v, t)$, possibly in some approximate sense? There is no universal answer to these questions in the current literature.

2.5 Validity of the Wigner–Poisson System

The Wigner–Poisson system is collisionless, in the same sense as is the Vlasov–Poisson system of classical plasma physics. In both models, the long-range interactions due to the self-consistent electrostatic potential are assumed to dominate over short-range collisional interactions between two or more particles. This statement can be made more precise [31]. Correlations between particles or equivalently collisions cannot be neglected if the average potential energy between two electrons become comparable to the average kinetic energy. As have been seen in the discussion on the classical and quantum energy coupling parameters of Sect. 1.4, we know the validity conditions for the collisionless approximation. For classical plasmas, it reads

$$\Gamma_C = \frac{U_{\text{pot}}}{K_C} = \frac{e^2 n_0^{1/3}}{\epsilon_0 \kappa_B T} \ll 1, \quad (2.70)$$

in terms of the classical coupling parameter Γ_C . On the other hand, for plasmas where the Fermi–Dirac statistics is unavoidable, collisions can be ignored provided

$$\Gamma_Q = \frac{U_{\text{pot}}}{K_Q} = \frac{e^2 n_0^{1/3}}{\epsilon_0 \kappa_B T_F} \sim \frac{me^2}{\epsilon_0 \hbar^2 n_0^{1/3}} \ll 1, \quad (2.71)$$

in terms of the quantum coupling parameter Γ_Q . As a consequence, for quantum plasmas ($T_F > T$) the collisionless approximation becomes better as the density increases.

When the condition $\Gamma_C \ll 1$ holds, the N -particle distribution can be factorized as a product of one-particle distribution functions satisfying Vlasov’s equation. Hence the Vlasov–Poisson system is the standard model to describe classical electrostatic plasmas in the collisionless approximation.

When the condition $\Gamma_Q \ll 1$ holds, a quantum electron gas can be described by the Wigner–Poisson system. In this case, the N -body Wigner function is expressed as a product of one-particle Wigner functions so that the Wigner–Poisson system is the natural model for collisionless quantum plasmas.

The previous results were derived in the limiting cases $T \gg T_F$ (classical) and $T \ll T_F$ (quantum degenerate). For intermediate temperatures, simple expressions for the coupling parameters are not available, but one must expect a smooth transition between the two regimes.

For electrons in metal, we have typically

$$n_0 \simeq 10^{29} \text{ m}^{-3}, \quad v_F \simeq 10^6 \text{ ms}^{-1}, \quad \omega_p \simeq 10^{16} \text{ s}^{-1}, \quad \lambda_F \simeq 10^{-10} \text{ m}. \quad (2.72)$$

These values yield a quantum coupling parameter of order unity. Allowing for the dimensionless constants, we have neglected and the different properties of metals, we realize that Γ_Q can be both smaller and larger than unity for typical metallic electrons [31].

Since $I_Q \sim 1$, apparently a collisionless model such as the Wigner–Poisson system could not be employed for metals. However, fortunately, the average rate of electron–electron collisions in such system is drastically reduced due to the Fermi–Dirac statistics. Indeed, in most cases of interest, for relatively low temperatures the vast majority of electrons is well below the Fermi energy. Since all lower levels are occupied, the exclusion principle forbids transitions except for the small electron population in a shell of thickness $\sim \kappa_B T$ around the Fermi surface, a phenomena know as Pauli blocking [2]. The e–e collision rate (inverse of the lifetime τ_{ee}) for such electrons is proportional to $\kappa_B T / \hbar$, as a consequence of the uncertainty principle energy \times time $\sim \hbar$. Since the fraction of electrons available to collisions is $\sim T / T_F$, one obtains

$$\frac{1}{\tau_{ee}} \sim \frac{1}{\hbar} \frac{\kappa_B T^2}{T_F}. \quad (2.73)$$

At room temperature, $\tau_{ee} \simeq 10^{-10}$ s, which is much larger than the typical collisionless time scale $\tau_p = \omega_p^{-1} \simeq 10^{-16}$ s. Therefore, for times smaller than τ_{ee} , the effect of e–e collisions can be safely neglected. In addition, it turns out that the typical relaxation time scale is $\tau_r \simeq 10^{-14}$ s, which is again significantly larger than τ_p . In summary, the ordering

$$\tau_p \ll \tau_r \ll \tau_{ee}, \quad (2.74)$$

implies that a collisionless (Wigner) model is appropriate for relatively short time scales [31].

Notice that not only very dense charged particle systems deserve quantum kinetic equations for their description. For instance, due to the ongoing miniaturization, even scarcely populated electronic systems such as resonant tunneling diodes [30] should be described in terms of quantum models. Indeed, the behavior of these ultra-small electronic devices relies on quantum diffraction effects as tunneling, making purely classical methods inappropriate. The nonlocal integro-differential potential term in (2.49) in the Wigner–Poisson system has been shown to be capable of the modeling of negative differential resistance, associated with tunneling [25]. Moreover, the collisionless approximation become more reasonable in view of the nanometric scale of the devices, 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 an operating frequency ω and a average time τ between collisions. For example, in resonant tunneling diodes one can find [30] potential barriers of the order $0.3 \text{ eV} \sim \hbar\omega$, implying an operating frequency $\omega \sim 10^{15} \text{ s}^{-1}$. Therefore, the Wigner–Poisson system is well suited for ballistic, collisionless processes in nanometric solid state devices, even at relatively low densities of order $n_0 \sim 10^{24} \text{ m}^{-3}$. Correspondingly, one finds a Fermi temperature $T_F \sim 40 \text{ K}$ much smaller than a typical room temperature $T \sim 300 \text{ K}$, justifying the nondegeneracy assumption and Maxwell–Boltzmann’s statistics.

2.6 Extensions to Include Correlation and Spin Effects

In spite of $df/dt \neq 0$, neither (2.49) nor (2.52) include collisions. Instead, the mean field (or Hartree) approximation is implicit in the Wigner–Poisson model, since its derivation assumed the factorization of the N -particle Wigner function $f^N = f^N(x_1, v_1, \dots, x_N, v_N, t)$ as a product of N identical one-particle Wigner functions, $f^N = f(x_1, v_1, t) \times \dots \times f(x_N, v_N, t)$. In this context, the scalar potential $\phi(x, t)$ comes from the collective field of the N electrons, just as in the classical theory. Allowing for correlations would result in a quantum BBGKY hierarchy.

In principle, a more detailed factorization taking into account the Pauli exclusion principle could have been employed. In this case, a Hartree–Fock term would be present in (2.49), see [24] for more details. However, frequently it is expedite to replace the complicated, nonlocal exchange-correlation terms by local phenomenological expressions, using the so-called adiabatic local density approximation (ALDA) [13, 33].

As remarked, quantum effects in a plasma (and in N -body systems in general) are unavoidable when the particle density is high enough. This can also be seen through the expansion parameter H in (2.52), which increase with density. To verify this, assume L_0 of the order of the mean inter-particle distance $n_0^{-1/3}$ and v_0 of the order of the thermal velocity v_T . Hence, $H \sim \hbar m_0^{1/3} / (m v_T)$, which is of order unity when the de Broglie wavelength $\lambda_B = \hbar / (m v_T)$ is comparable to the mean inter-particle separation. In this case, there will be a significant overlap of the wave packets associated with each electron, so that the Newtonian approximation breaks down. On the other hand, a collisionless model for quantum plasmas becomes more accurate for higher densities, see the quantum coupling parameter Γ_Q in (2.71). We use this conclusion as a methodological argument in favor of the Wigner–Poisson system, even if the underlying Fermi–Dirac statistics is not included in (2.49) and (2.51). We also note that the classical energy coupling parameter usually Γ_C in (2.70) plays a marginal rôle in quantum plasmas.

On the other hand, it is worth to say that the Wigner–Poisson system is employed in the semiconductor literature where typically the particle densities are not so high. Except for short-time ballistic phenomena, in such cases, it is crucial to improve the model by means of adequate collision operators [30]. For instance, in a resonant tunneling diode quantum effects are noticeable thanks to the smallness of the system, so that the basic characteristic length is the size of the device rather than the average inter-particle distance. Mathematically, the size of the system manifests, for example, through the boundary conditions.

In recent years [1, 9, 28], much attention has been devoted to the Wigner–Fokker–Planck equation

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} - \int dv' K_\phi[\phi | v' - v, x, t] f(v', x, t) = L_{\text{QFP}}[f], \quad (2.75)$$

for the modeling of quantum dissipation, with

$$L_{\text{QFP}}[f] = \frac{D_{pp}}{m^2} \frac{\partial^2 f}{\partial v^2} + \frac{\eta}{m} \frac{\partial}{\partial v} (v f) + \frac{2}{m} D_{pq} \frac{\partial^2 f}{\partial v \partial x} + D_{qq} \frac{\partial^2 f}{\partial x^2} \quad (2.76)$$

acting as a collision term. In this case, it is assumed an open quantum system interacting with a heat bath of harmonic oscillators. Here,

$$D_{pp} = \eta \kappa_B T, \quad D_{pq} = \frac{\eta \Omega \hbar^2}{12 \pi m \kappa_B T}, \quad D_{qq} = \frac{\eta \hbar^2}{12 m^2 \kappa_B T} \quad (2.77)$$

are phenomenological constants related to the interactions, where η is the damping coefficient of the bath, T is the bath temperature and Ω is the cut-off frequency of the reservoir oscillators. Physically, the heat bath of harmonic oscillators can be realized, for example, in terms of the phonons propagating in a crystal lattice.

Notice that for homogeneous equilibrium ($\partial f / \partial x = 0$) or for vanishing quantum effects, the Maxwellian $f = f_M \sim \exp(-v^2/2 v_T^2)$, $v_T^2 = \kappa_B T / m$ belongs to the kernel of the collision operator (2.76), or

$$L_{\text{QFP}}[f_M] = 0. \quad (2.78)$$

Actually this comes with no surprise since the Wigner–Fokker–Planck model is derived [1, 9] on the assumption of classical statistics, that is, no spin degrees of freedom. In addition, if D_{pq} and D_{qq} are set to zero the Caldeira–Legget [7] model is recovered. However, importantly the Wigner–Fokker–Planck collision operator can be put in the Lindblad form [27] provided

$$D_{pp} D_{qq} \geq D_{pq}^2 + \frac{\hbar^2 \eta^2}{16 m^2} \quad \text{or} \quad \hbar \Omega \leq \sqrt{3} \pi \kappa_B T, \quad (2.79)$$

the last inequality holding for $\eta \neq 0$. Accordingly, it can be shown that the associated density matrix operator preserves positivity under time-evolution, a feature not satisfied by the Caldeira–Legget model.

Promising as it is, the Wigner–Fokker–Planck model did not apply to dense quantum plasma astrophysical environments, where the fermion statistics play a significant rôle. Therefore, the inclusion of suitable dissipation mechanisms is a challenge in quantum plasma physics.

2.7 High Frequency Longitudinal Waves

For any plasma, the propagation of linear waves is an essential issue. Assuming a wave with wave number k and frequency ω propagating in a plasma described by the Wigner–Poisson system (2.49) and (2.51), set

$$f(x, v, t) = f_0(v) + f_1(v) \exp(i[kx - \omega t]), \quad (2.80)$$

$$\phi = \phi_1 \exp(i[kx - \omega t]), \quad (2.81)$$

for first-order disturbances f_1, ϕ_1 . It is supposed an equilibrium Wigner function $f = f_0(v)$ such that $\int dv f_0(v) = n_0$ and a zero equilibrium electrostatic potential.

Linearizing (2.49) and (2.51) it follows

$$-i(\omega - kv)f_1(v) = \left(f_0 \left(v + \frac{\hbar k}{2m} \right) - f_0 \left(v - \frac{\hbar k}{2m} \right) \right) \phi_1, \quad (2.82)$$

$$-k^2 \phi_1 = \frac{e}{\epsilon_0} \int dv f_1(v). \quad (2.83)$$

This linear homogeneous system for f_1, ϕ_1 admit nontrivial solutions if and only if

$$\epsilon \equiv 1 - \frac{m\omega_p^2}{n_0\hbar k^2} \int dv \frac{f_0[v + \hbar k/(2m)] - f_0[v - \hbar k/(2m)]}{kv - \omega} = 0. \quad (2.84)$$

Here $\omega_p = (n_0 e^2 / m\epsilon_0)^{1/2}$ is the plasma frequency.

For the dispersion properties only, (2.84) can be understood in the principal value sense. In addition, it is convenient to change integration variables so as to rewrite the permittivity ϵ as

$$\epsilon = 1 - \frac{\omega_p^2}{n_0} \int dv \frac{f_0(v)}{(\omega - kv)^2 - \hbar^2 k^4 / (4m^2)}. \quad (2.85)$$

Further, it is useful [14] to introduce the rescaling

$$F = \frac{\omega_p f_0}{n_0 k}, \quad u = \frac{kv}{\omega_p}, \quad \Omega = \frac{\omega}{\omega_p}, \quad (2.86)$$

so that

$$\epsilon = 1 - \frac{1}{\Omega^2} \int \frac{du F(u)}{(1 - u/\Omega)^2 - \Omega_q^2 / \Omega^2} = 0, \quad (2.87)$$

where $\int du F(u) = 1$ and it was defined

$$\Omega_q^2 = \frac{\hbar^2 k^4}{4m^2 \omega_p^2}. \quad (2.88)$$

For high frequency oscillations, we can consider expanding the integrand retaining up to $O(\Omega_q^2 / \Omega^2, \langle u^2 \rangle / \Omega^2)$ terms, (2.87) becomes

$$\epsilon \simeq 1 - \frac{1}{\Omega^2} \left(1 + \frac{3\langle u^2 \rangle + \Omega_q^2}{\Omega^2} \right) = 0. \quad (2.89)$$

In (2.89), $\langle u^2 \rangle = \int du F(u) u^2$. For simplicity, $\int du F(u) u = 0$ was assumed, which holds for instance for symmetric equilibria.

Solving (2.89) by successive approximations, the result is

$$\Omega^2 = 1 + 3 \langle u^2 \rangle + \Omega_q^2 \quad (2.90)$$

or

$$\omega^2 = \omega_p^2 + 3k^2 \langle v^2 \rangle + \frac{\hbar^2 k^4}{4m^2}, \quad (2.91)$$

where $\langle v^2 \rangle = \int dv f_0(v) v^2 / n_0$. Equation (2.91) is the Bohm–Pines dispersion relation [5], the quantum counterpart of the Bohm–Gross dispersion relation of classical high frequency longitudinal plasma waves [4].

Equation (2.91) describes quantum Langmuir waves and is correct no matter the form of the equilibrium Wigner function, as far as the high frequency hypothesis is valid. In the case [24] of zero velocity dispersion ($f_0(v) = n_0 \delta(v)$) one has

$$\omega^2 = \omega_p^2 + \frac{\hbar^2 k^4}{4m^2}. \quad (2.92)$$

Here, it is referred to “zero velocity dispersion” rather than to “zero-temperature” to not confound with, for instance, a zero-temperature Fermi gas, where $\langle v^2 \rangle \neq 0$ in consequence of the exclusion principle.

For the imaginary part of the frequency, it is useful to rewrite (2.84) according to

$$\varepsilon = 1 - \frac{m \omega_p^2}{n_0 \hbar k^2} \left(\int_{L_+} \frac{dv f_0(v)}{k[v - \hbar k/(2m)] - \omega} - \int_{L_-} \frac{dv f_0(v)}{k[v + \hbar k/(2m)] - \omega} \right) = 0, \quad (2.93)$$

where the velocity integrals are performed with Landau contours L_{\pm} passing under the poles at $v = \omega/k \pm \hbar k/(2m)$. Equation (2.93) can be used [24,35] as the starting point for the discussion of the quantum Landau damping, the quantum counterpart of the collisionless damping present in classical plasmas.

From (2.93), assuming that the damping or growth rate γ is small and repeating the procedure for classical plasmas (see Problem 2.7), we get

$$\gamma = \frac{\pi \omega_p^3}{4 n_0 k^2} \left(\frac{f_0[\omega/k + \hbar k/(2m)] - f_0[\omega/k - \hbar k/(2m)]}{\hbar k/(2m)} \right), \quad (2.94)$$

where ω follows from (2.90). Hence, the damping (or growth) rate of quantum Langmuir waves is a finite-difference version of the classical growth rate γ_{cl} , which is obtained from (2.94) in the formal limit $\hbar \rightarrow 0$,

$$\gamma_{cl} = \frac{\pi \omega_p^3}{2 n_0 k^2} \frac{df_0}{dv} \left(v = \frac{\omega}{k} \right). \quad (2.95)$$

It is relevant to remark that from (2.94), a particular class of stationary solutions such that $\gamma = 0$ is given by any function $f_0(v)$ which is a periodic in velocity space, with period $\hbar k/m$:

$$f_0\left(\frac{v+\hbar k}{2m}\right) - f_0\left(\frac{v-\hbar k}{2m}\right) = 0. \quad (2.96)$$

Assuming $f_0(v) \sim \exp(i\alpha v)$ in (2.96), with α to be determined, we obtain the characteristic equation $\sin(\alpha\hbar k/(2m)) = 0$. Hence, an exact equilibrium solution is the linear combination, or Fourier series

$$f_0(v) = a_0 + \sum_{n=1}^{\infty} a_n \cos\left(\frac{2\pi n v}{\lambda_v}\right) + \sum_{n=1}^{\infty} b_n \sin\left(\frac{2\pi n v}{\lambda_v}\right), \quad (2.97)$$

where a_n, b_n are arbitrary real constants and $\lambda_v = \hbar k/m$. Notice the singular character of the quantum oscillations, whose “wavelength” of the fundamental mode ($n = 1$) in velocity space tends to zero as $\hbar \rightarrow 0$. The solution given by (2.97) represents periodic oscillations in velocity space. This is in sharp contrast to the classical stationary solution which points to the formation of a plateau ($df_0/dv = 0$) at the resonance, see (2.95). The oscillating character of quantum plasma equilibria has been predicted in terms of a quantum quasilinear theory and numerically verified [16].

The treatment of nonlinear phenomena in the Wigner–Poisson framework is rather involved, with few known analytic results. For instance, a few classes of exact nonlinear stationary solution is available [15]. The most expedite route toward nonlinear quantum plasmas is by means of hydrodynamic formulations, as we start to verify in the next chapter.

Problems

2.1. Use $v \exp(-imvs/\hbar) = (i\hbar/m)(\partial/\partial_s) \exp(-imvs/\hbar)$ and integration by parts assuming decaying or periodic boundary conditions to check (2.3).

2.2. Check the last equality in (2.7) as well as (2.8).

2.3. Derive (2.52) starting from (2.49).

2.4. Work out (2.56) and (2.59) for a Gaussian shaped Wigner function $f = A \exp(-v^2/\delta v^2 - x^2/\delta x^2)$, $A = \text{cte}$. Show that $m\delta v\delta x \geq \hbar$.

2.5. Expand the equation of motion for the one-particle Wigner function in one spatial dimension up to fourth-order in the dimensionless quantum parameter H . Discuss the properties of quantum robust solutions, defined as the Wigner functions for which the quantum effects vanish up to $O(H^5)$.

2.6. Show that the Maxwellian belongs to the kernel of the Wigner–Fokker–Planck collision operator.

2.7. Consult a standard plasma textbook where the damping rate of Langmuir waves is derived and repeat the procedure in the quantum case, to get (2.94) using (2.93).

References

1. Arnold, A., López, J. L., Markowich, P., Soler, J.: An analysis of quantum Fokker-Planck models: a Wigner function approach. *Rev. Mat. Iberoamericana* **20**, 771–814 (2004)
2. Ashcroft, N. W. and Mermin, N. D.: Solid state physics. Saunders College Publishing, Orlando (1976)
3. Bogoliubov, N. N.: Kinetic equations. *J. Exp. Theor. Phys.* **16**, 691–702 (1946)
4. Bohm, D. and Gross, E.: Theory of plasma oscillations. A. Origin of medium-like behavior. *Phys. Rev.* **75**, 1851–1864 (1949)
5. Bohm, D., Pines, D.: A collective description of electron interactions: III. Coulomb interactions in a degenerate electron gas. *Phys. Rev.* **92**, 609–625 (1953)
6. Born, M., Green, H. S.: A general kinetic theory of liquids I. The molecular distribution functions. *Proc. Roy. Soc. A* **188**, 10–18 (1946)
7. Caldeira, A. O., Leggett, A. J.: Path integral approach to quantum Brownian motion. *Physica A* **121**, 587–616 (1983)
8. Carruthers, P., Zachariasen, F.: Quantum collision theory with phase-space distributions. *Rev. Mod. Phys.* **55**, 245–285 (1983)
9. Castella, F., Erdős, L., Frommlet, F., Markowich, P.: Fokker-Planck equations as scaling limits of reversible quantum systems. *J. Stat. Phys.* **100**, 543–601 (2000)
10. DiVentra, M.: Electrical Transport in Nanoscale Systems. Cambridge, New York (2008)
11. Glauber, R. J.: Coherent and incoherent states of the radiation field. *Phys. Rev.* **131**, 2766–2788 (1963)
12. Glauber, R.J.: Optical coherence and photon statistics. In: Dewitt, C., Blandin, A., Cohen-Tannoudji, C. (eds.) *Quantum Optics and Electronics*, pp. 63–185, Gordon and Breach, New York (1965)
13. Gusev, G. M., Quivy, A. A., Laman, T. E., Leite, J. R., Bakarov, A. K., Topov, A. I., Estibals, O., Portal, J. C.: Magnetotransport of a quasi-three-dimensional electron gas in the lowest Landau level. *Phys. Rev. B* **65**, 205316–205325 (2002)
14. Haas, F.: On quantum plasma kinetic equations with a Bohmian force. *J. Plasma Phys.* **76**, 389–393 (2010)
15. Haas, F. and Shukla, P. K.: Nonlinear stationary solutions of the Wigner and Wigner–Poisson equations. *Phys. Plasmas* **15**, 112302–112302-6 (2008)
16. Haas, F., Eliasson, B., Shukla, P. K. and Manfredi, G.: Phase-space structures in quantum-plasma wave turbulence. *Phys. Rev. E* **78**, 056407–056414 (2008)
17. Haug, H. J. W., Jauho, A. P.: *Quantum Kinetics in Transport and Optics of Semiconductors*. Springer, Berlin-Heidelberg (2008)
18. Hillery, M., O’Connell, R. F., Scully, M. O., Wigner, E. P.: Distribution functions in physics - fundamentals. *Phys. Rep.* **106**, 121–330 (1990)
19. Husimi, K.: Some formal properties of the density matrix. *Prog. Phys. Math. Soc. Japan* **22**, 264–314 (1940)
20. Jungel, A.: *Transport Equations for Semiconductors*. Springer, Berlin-Heidelberg (2009)
21. Kadanoff, L.P., Baym, G.: *Quantum Statistical Mechanics: Green’s Function Methods in Equilibrium and Non-Equilibrium Problems*. Benjamin, New York (1962)
22. Kirkwood, J. G.: Quantum statistics of almost classical assemblies. *Phys. Rev.* **44**, 31–37 (1933)
23. Kirkwood, J. G.: The statistical mechanical theory of transport processes I. General theory. *J. Chem. Phys.* **14**, 180–201 (1946)
24. Klimontovich Y. and Silin, V. P.: The spectra of systems of interacting particles. In: Drummond, J. E. (ed.) *Plasma Physics*, pp. 35–87, McGraw-Hill, New York (1961)
25. Klusdahl, N. C., Krivan, A. M., Ferry, D. K., Ringhofer, C.: Self-consistent study of the resonant tunneling diode. *Phys. Rev. B.* **39**, 7720–7735 (1989)
26. Lee, H.: Theory and application of the quantum phase-space distribution functions. *Phys. Rep.* **259**, 147–211 (1995)

27. Lindblad, G.: On the generators of quantum dynamical semigroups. *Commun. Math. Phys.* **48**, 119–130 (1976)
28. López, J. L.: Nonlinear Ginzburg-Landau-type approach to quantum dissipation. *Phys. Rev. E* **69**, 026110–026125 (2004)
29. Markowich, P. A.: On the equivalence of the Schrödinger and the quantum Liouville equations. *Math. Meth. in the Appl. Sci.* **11**, 459–469 (1989)
30. Markowich, P. A., Ringhofer, C. A., Schmeiser, C.: *Semiconductor Equations*. Springer, Wien (1990)
31. Manfredi, G., Haas, F.: Self-consistent fluid model for a quantum electron gas. *Phys. Rev. B* **64**, 075316–075323 (2001)
32. Mehta, C. L.: Phase-space formulation of the dynamics of canonical variables. *J. Math. Phys.* **5**, 677–686 (1964)
33. Santer, M., Mehlig, B., Moseler, M.: Optical response of two-dimensional electron fluids beyond the Kohn regime: strong nonparabolic confinement and intense laser light. *Phys. Rev. Lett.* **89**, 266801–266804 (2002)
34. Sudarshan, E. C. G.: Equivalence of semiclassical and quantum mechanical descriptions of statistical light beams. *Phys. Rev. Lett.* **10**, 277–279 (1963)
35. Suh, N., Feix, M. R. and Bertrand, P.: Numerical simulation of the quantum Liouville-Poisson system. *J. Comput. Phys.* **94**, 403–418 (1991)
36. Tatarskii, V. I.: The Wigner representation of quantum mechanics. *Sov. Phys. Usp.* **26**, 311–327 (1983)
37. Weyl, H.: Quantenmechanik und gruppentheorie. *Z. Phys.* **46**, 1–46 (1927)
38. Wigner, E.: On the quantum correction for thermodynamic equilibrium. *Phys. Rev.* **40**, 749–759 (1932)
39. Yvon, J.: *La Théorie Statistique des Fluides*. Hermann, Paris (1935)



<http://www.springer.com/978-1-4419-8200-1>

Quantum Plasmas

An Hydrodynamic Approach

Haas, F.

2011, XIV, 206 p., Hardcover

ISBN: 978-1-4419-8200-1