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Expansion of a quantum electron gas

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The expansion of a quantum electron gas (non-relativistic, no spin) is investigated via the one-particle Schrödinger–Poisson model. Classically, the nonlinear term enhances the formation of a very regular asymptotic state. By means of rescaling methods, we conjecture that the quantum asymptotic solution is identical to the classical one. Subsequent numerical simulations confirm the above conjecture and define precisely the way in which the classical limit is approached. The numerical results are supported by several analytical calculations: in particular, it is proved that the rescaled equations can be written in a way such that a vanishing Planck's constant appears. This trick allows us to evaluate the quantum correction terms. Finally, we show the existence of an analytical solution, the Wigner transform of which exactly corresponds to the classical solution.

1. Introduction

In recent years there has been increasing interest in models that account for quantum effects in transport phenomena. From a practical point of view, much work has aimed at modelling the features of small semiconductor devices, in which the de Broglie wavelength of the charge carriers is of the same order of magnitude as the size of the device. However, quantum transport equations present some theoretical interest *per se*, which justifies the study of a few idealized situations such as the expansion-into-vacuum problem.

Several approaches to the modelling of quantum plasmas are already available – the most widely used models are based on either the Wigner or the Schrödinger equation to describe the dynamics of the electrons, whereas the electrostatic interactions are treated self-consistently via the Poisson equation. Because of the coupling with the Poisson equation, both models are highly nonlinear, so that analytical investigations soon become a formidable task: we believe that a combination of analytical and numerical tools can be an efficient approach to this kind of problems.

In the Wigner representation (for a review see Tatarskii 1983), quantum mechanics is expressed in a phase-space formalism, in which the quasi-probability density (called the Wigner function) is unambiguously derived from the Schrödinger wavefunction. Such a density obeys an evolution equation that bears some analogy with the classical Liouville equation. Unfortunately, the Wigner function cannot be regarded as a true probability density, since it exhibits a few 'unpleasant' features (including non-positivity), but can nevertheless be used operationally, although with some caution, to calculate the evolution of any dynamical quantity. A remarkable advantage of the

Wigner formalism is that both pure and mixed states are treated on the same basis, the only difference lying in the choice of the initial condition.

Several codes have recently been proposed for solving the Wigner–Poisson system, both in the Eulerian formalism (using a distribution function – Suh, Feix & Bertrand 1991) and in the Lagrangian formalism (following the trajectories of pseudo-particles – Arnold & Markovich 1991; Arnold & Nier 1992). It should be noted, however, that the philosophy of particle codes is, in principle, ill suited to treating a quantum-mechanical problem, since the very concept of a classical trajectory loses its meaning. In fact, in such codes one is obliged to reconstruct a distribution function in order to compute the acceleration term, thus losing most of the advantages of classical Lagrangian codes. For this reason, we believe that Eulerian codes are definitely more appropriate for simulating quantum-mechanical evolutions in phase space.

On the other hand, the Schrödinger–Poisson system has long been used in its stationary version, in order to study the energy spectrum of electrons in semiconductor devices (Cruz Serra & Aren Santos 1991; Kerkhoven *et al.* 1990). However, the existing literature on the time-dependent Schrödinger–Poisson system is much narrower. In several papers (Bertrand *et al.* 1980; Nguyen *et al.* 1985) the authors have investigated the classical limit in order to recover the evolution of a classical plasma. The main idea underlying this approach is that the Schrödinger equation depends only on the co-ordinate variables, whereas a correct treatment of a classical plasma involves the whole phase space, thus requiring a considerably stronger numerical effort. As a matter of fact, it turns out that, to obtain a significant reduction of the numerical effort, one has to accept the presence of finite quantum effects.

More recently, the time-dependent Schrödinger–Poisson system has been used in the study of carrier transport in very small semiconductor devices (Yalabik *et al.* 1989). Here, we revisit this model to investigate the expansion of a quantum electron gas into vacuum, under the action of its own self-consistent field, in planar geometry.

Although the study of practical devices involves a more complex geometry, such a situation is interesting in principle, since the corresponding classical expansion possesses a simple well-known solution for $t \to \infty$ (Burgan *et al.* 1983). Comparison between the classical and quantum solutions will be the main purpose of this paper. We shall see, in fact, that the classical solution acts as an asymptotic attractor, so that for $t \to \infty$ the system spontaneously approaches its classical limit.

We shall restrict ourselves to one-dimensional problems, for which the Schrödinger–Poisson system is

$$\left.\begin{aligned} i\hbar\frac{\partial\psi}{\partial t} &= -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + eV\psi, \\ \frac{\partial^2 V}{\partial x^2} &= -\frac{Ne}{\varepsilon_0}|\psi|^2, \end{aligned}\right\} \qquad (1)$$

$$\int |\psi|^2\,dx = 1, \quad \psi(x, t=0) = \psi_0(x)$$

where $\hbar$ is Planck's constant, ε_0 the dielectric constant in vacuum, e and m the electron charge and mass respectively, and N the total number of electrons per

unit area. All the parameters in (1) can be eliminated by simple dimensional analysis. The dimensionless variables (indicated by a tilde) are given by the following relations:

$$\left.\begin{aligned} \tilde{x} &= \frac{x}{\hbar^{\frac{2}{3}} m^{-\frac{1}{3}} N^{-\frac{1}{3}} \varepsilon_0^{\frac{1}{3}}} e^{-\frac{2}{3}}, \quad \tilde{t} = \frac{t}{\hbar^{\frac{1}{3}} m^{\frac{1}{3}} N^{-\frac{2}{3}} \varepsilon_0^{\frac{2}{3}}} e^{-\frac{4}{3}}, \\ \tilde{\psi} &= \frac{\psi}{\hbar^{-\frac{1}{3}} m^{\frac{1}{6}} N^{\frac{1}{6}} \varepsilon_0^{-\frac{1}{6}} e^{\frac{1}{3}}}, \quad \tilde{V} = \frac{V}{\hbar^{\frac{2}{3}} m^{-\frac{1}{3}} N^{\frac{2}{3}} \varepsilon_0^{-\frac{2}{3}} e^{\frac{1}{3}}}. \end{aligned}\right\} \tag{2}$$

In the following we shall take $\hbar = m = \varepsilon_0 = e = N = 1$, and drop tildes for the sake of simplicity.

In our approach a one-particle wave function is used to describe a system of N particles. This is, of course, an approximation, which is analogue to the Vlasov approximation for classical plasmas, where a system of N particles is described by a one-particle probability distribution. It implies neglecting individual interactions between particles, while taking into account collective interactions, via the Poisson law. In addition, no spin or relativistic phenomena are considered.

Another, more mathematical, aim will be the generalization of the so-called rescaling transformations (see e.g. Burgan *et al.* 1978, 1983) to the Schrödinger formalism: these techniques will suggest conjectures on the structure of the solution, and, at the same time, facilitate the numerical integration. As a general method, rescaling seems to be a powerful tool in the numerical and analytical treatment of nonlinear equation, well beyond the particular case treated here. It has been used to investigate very different problems, such as the expansion of a two-species plasma (Manfredi, Mola & Feix 1993), nonlinear diffusion (Zrineh *et al.* 1987), gravitational hydrodynamics (Bouquet & Feix 1982) and nonlinear ordinary differential equations (Besnard *et al.* 1983).

Finally, we remark that a popular model in nonlinear plasma physics is the nonlinear Schrödinger equation (NLS), which is (see Ablowitz & Segur 1981)

$$i\frac{\partial \psi}{\partial t} = -\frac{1}{2}\frac{\partial^2 \psi}{\partial x^2} + \alpha |\psi|^2 \psi. \tag{3}$$

Consider now the equation

$$i\frac{\partial \psi}{\partial t} = -\frac{1}{2}\frac{\partial^2 \psi}{\partial x^2} + \left[\int_{-\infty}^{\infty} |\psi(x',t)|^2 G(x,x')\,dx'\right]\psi(x,t). \tag{4}$$

We immediately recognize that our Schrödinger–Poisson model is obtained by taking $G(x,x') = \frac{1}{2}|x-x'|$, while $G(x,x') = \alpha\delta(x-x')$ provides the usual NLS. Note the non-local character of the nonlinear interacting term in the Schrödinger–Poisson model, contrasted with the local character of this term in the NLS.

The present paper is structured as follows. In §2 we introduce the rescaling transformation in the classical domain, and recall the features of the classical electron-gas expansion. In §3 we generalize the rescaling to the Schrödinger equation, and prove the main results for the quantum expansion either numerically or analytically. In §4 we introduce the Wigner formalism, which is used throughout §5 to study the classical–quantum correspondence for our system. We give our conclusions in §6.

2. The classical expansion and rescaling

The problem of a freely expanding electron gas was investigated classically by Burgan *et al.* (1983). The dynamics of the electrons was treated through the Vlasov equation, coupled self-consistently to the Poisson equation. The system is (in normalized units)

$$\left.\begin{aligned} &\frac{\partial f}{\partial t}+v\frac{\partial f}{\partial x}+E\frac{\partial f}{\partial v}=0,\\ &\frac{\partial E}{\partial x}=\int_{-\infty}^{\infty} f(x,v,t)\,dv, \end{aligned}\right\} \tag{5}$$

where $E(x,t)=-\partial V/\partial x$ is the electric field and $f(x,v,t)$ the phase-space density. Since no external confining potential is present, the electron gas tends to expand to infinity under the action of its own repulsive self-consistent field. It is therefore convenient, both analytically and numerically, to perform a transformation (called rescaling) so that, in the new variables, the system is confined.

We introduce new space, time and velocity variables, as well as a rescaled distribution function, defined by

$$\left.\begin{aligned} x &= C(t)\,\xi,\\ dt &= A^2(t)\,d\vartheta,\\ v &= \frac{dx}{dt}=C\frac{d\xi}{d\vartheta}\frac{d\vartheta}{dt}+\xi\frac{dC}{dt}=\eta\frac{C}{A^2}+\xi\frac{dC}{dt}, \quad \eta=\frac{d\xi}{d\vartheta},\\ f(x,v,t) &= G(t)F(\xi,\eta,\vartheta), \end{aligned}\right\} \tag{6}$$

where $A(t)$, $C(t)$ and $G(t)$ are three arbitrary functions, with the sole constraint of being regular and non-zero over $[0,\infty]$.

By substituting (6) into (5), one can derive a rescaled Vlasov–Poisson system, which, in the most general case, is rather complicated. However, upon assuming for $A(t)$, $C(t)$ and $G(t)$ a time dependence of the form $(1+\Omega t)^\beta$, (where $\beta\in\mathbb{R}$, and $\Omega>0$ is an arbitrary frequency characterizing the transformation), the rescaled system can be made considerably simpler and, above all, time-independent. In order to do so, one has to choose

$$A(t)=(1+\Omega t)^{\frac{1}{2}}, \quad C(t)=(1+\Omega t)^2, \quad G(t)=(1+\Omega t)^{-3}. \tag{7}$$

The form of $C(t)$ tells us that the electron gas expands as t^2, that is, with constant acceleration.

The rescaled Vlasov–Poisson then becomes

$$\left.\begin{aligned} &\frac{\partial F}{\partial\vartheta}+\eta\frac{\partial F}{\partial\xi}+\frac{\partial}{\partial\eta}[(\varepsilon-2\Omega^2\xi-3\Omega\eta)F]=0,\\ &\frac{\partial\varepsilon}{\partial\xi}=\int F\,d\eta, \end{aligned}\right\} \tag{8}$$

in which $\varepsilon(\xi,\vartheta)=E(x,t)$.

The rescaling transformation has introduced two new terms in the Vlasov equation, namely a confining linear force $(-2\Omega^2\xi)$ and a friction $(-3\Omega\eta)$. Owing

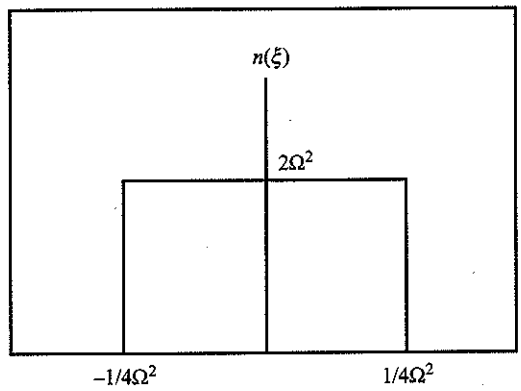

FIGURE 1. Theoretical profile of the spatial density $n(\xi)$ for the classical solution in the rescaled space.

to the presence of such terms, it is easy to deduce the asymptotic state of the system (8). Such a system will simply relax, in (ξ, η) space, to a motionless stationary state (that is, $\eta = 0$) for which the self-consistent field exactly cancels the external field (that is, $\varepsilon = 2\Omega^2\xi$). This is possible only for a spatially uniform density, equal to $n_0 = 2\Omega^2$ in the interval $[-1/4\Omega^2, 1/4\Omega^2]$, and zero outside, as plotted in figure 1.

The asymptotic solution of (8) is therefore given by the following relations (for more details see Burgan *et al.* 1983):

$$E(x,t) = \frac{2x}{t^2} \quad \text{as } t \to \infty, \tag{9}$$

$$f(x,v,t) = \frac{2}{t^2}\delta\left(v - \frac{2x}{t}\right) \quad \text{as } t \to \infty, \tag{10}$$

where δ is the Dirac delta function. The important property of the solution (9), (10) is that it is a universal attractor, in the sense that all initial conditions relax asymptotically to give such a configuration.

The previous discussion indicates that the evolution of our system is not symmetric in time. This fact is explicitly contained in the rescaled Vlasov–Poisson equations: indeed, the presence of a friction term clearly reveals the existence of a privileged direction in the flow of time, going from an arbitrary initial condition towards the motionless asymptotic state. This corresponds, in real space, to an arrow of time pointing in the direction in which the system expands. Of course, one can always prepare some very special initial condition so that the system initially contracts. Nevertheless, for large enough times, the arrow of time dominates, and the system will expand.

3. The quantum expansion

We now investigate the quantum treatment of the electron-gas expansion, for which we make use of the self-consistent Schrödinger–Poisson system (1), the physical assumptions underlying which have already been stated in §1. Since the rescaling technique has turned out to be very fruitful in the classical domain, we should like to apply it also to the quantum-mechanical problem.

However, this is not trivial, for the transformation (6) is not necessarily a canonical one: in particular, the 'good' transformation that led to the time-independent rescaled Vlasov–Poisson system (8) introduced a friction term, which is of course not derivable from a Hamiltonian. On the other hand, quantum mechanics requires a Hamiltonian formalism to be used. In fact, the transformation (6) can be rendered canonical without any loss of generality, upon using the following trick. We define a 'time-dependent mass' $\mu(t)$ and a 'rescaled momentum' Π as follows:

$$\mu(t) = \frac{C^2}{A^2}; \quad \Pi = \mu(t)\,\eta. \tag{11}$$

Substitution of (11) into (6) yields

$$\left.\begin{aligned} x &= C(t)\,\xi, \\ p &= \frac{\Pi}{C(t)} + \dot{C}(t)\,\xi, \\ dt &= A^2(t)\,d\vartheta, \end{aligned}\right\} \tag{12}$$

where $p = v$, since $m = 1$; a dot stands for differentiation with respect to t.

The transformation (12) is a linear, point canonical transformation, as can easily be verified by evaluating the Poisson brackets $[\xi, \Pi] = [x, p] = 1$. It is also a kind of 'generalized' canonical transformation, since it is explicitly time-dependent. The type-two generating function (Goldstein 1980) for the transformation (12) is given by

$$F_2(x, \Pi, t) = \frac{1}{2}\frac{\dot{C}}{C}x^2 + \frac{x\Pi}{C}. \tag{13}$$

Thus, if a system is described by the Hamiltonian

$$H(x, p, t) = \tfrac{1}{2}p^2 + V(x, t), \tag{14}$$

the transformed Hamiltonian $\bar{H}$ will be

$$\bar{H}(x, \Pi, \vartheta) = A^2\left[H(x, p, t) + \frac{\partial F_2}{\partial t}\right] = \frac{A^2}{C^2}\frac{\Pi^2}{2} + A^2C\,[\bar{V}(\xi, \vartheta) + \tfrac{1}{2}\ddot{C}\xi^2]. \tag{15}$$

In (15) we have also rescaled the potential, with

$$V(x, t) = C(t)\,\bar{V}(\xi, \vartheta), \tag{16}$$

so that the Poisson equation is left invariant in the new variables.

Quantization of the Hamiltonian (15) is straightforward. By means of the usual correspondence rules between position and momentum and their respective operators, one obtains the rescaled Schrödinger equation

$$i\frac{\partial\bar{\psi}}{\partial\vartheta} = -\frac{A^2}{C^2}\frac{1}{2}\frac{\partial^2\bar{\psi}}{\partial\xi^2} + A^2C\bar{V}\bar{\psi} + \tfrac{1}{2}A^2C\ddot{C}\xi^2\bar{\psi}, \tag{17}$$

where $\bar{\psi}(\xi, \vartheta)$ is the new wave function.

The preceding formula is a slight generalization of the rescaling given in Burgan *et al.* (1978), where $A = C$ was always chosen.

We still have to express the relation between the old and new wave functions. In order to do this, we first present a formal derivation, which perhaps provides deeper physical insight. Let us write ψ and $\bar{\psi}$ as

$$\left.\begin{aligned}\psi(x,t) &= [n(x,t)]^{\frac{1}{2}}\exp[iS(x,t)],\\ \bar{\psi}(\xi,\vartheta) &= [\bar{n}(\xi,\vartheta)]^{\frac{1}{2}}\exp[i\bar{S}(\xi,\vartheta)],\end{aligned}\right\} \tag{18}$$

$n^{\frac{1}{2}}$ and $\bar{n}^{\frac{1}{2}}$ being the amplitudes, and S and $\bar{S}$ the phases. The normalization condition imposes

$$|\psi|^2\,dx = |\bar{\psi}|^2\,d\xi. \tag{19}$$

Using (12) and (19), one gets the relation between the amplitudes

$$\bar{n}(\xi,\vartheta) = C(t)\,n(x,t). \tag{20}$$

As to the phases S and $\bar{S}$, we recall that the phase of the wave function is related to the classical momentum through

$$p = \frac{\partial S}{\partial x}, \quad \Pi = \frac{\partial \bar{S}}{\partial \xi}.$$

Note that these relations are valid not only in the classical limit, since now we regard p as a function of position.

Substituting the above relations into the second of (12) and integrating gives

$$S = \bar{S} + \frac{1}{2}\frac{\dot{C}}{C}x^2, \tag{21}$$

up to an immaterial additive constant. From (20) and (21) we can write the relation between the wave functions:

$$\psi(x,t) = \frac{1}{C^{\frac{1}{2}}}\exp\left(i\frac{\dot{C}x^2}{2C}\right)\bar{\psi}(\xi,\vartheta). \tag{22}$$

Note that (22) represents a unitary transformation of the wavefunction.

The suspicious reader may verify that, by defining the most general transformation between the wave functions as

$$\psi(x,t) = B(t)\exp[iK(t)\varphi(x)]\,\bar{\psi}(\xi,\vartheta), \tag{23}$$

where $B(t)$, $K(t)$ and $\varphi(x)$ are arbitrary real functions, and substituting (23) into the first of (1), one does obtain the rescaled Schrödinger equation (17) only if $B(t) = C^{-\frac{1}{2}}$ and $K(t)\varphi(x) = \dot{C}x^2/2C$.

The new Schrödinger–Poisson system is

$$\left.\begin{aligned} i\frac{\partial\bar{\psi}}{\partial\vartheta} &= -\frac{A^2}{2C^2}\frac{\partial^2\bar{\psi}}{\partial\xi^2} + A^2C(\bar{V}+\tfrac{1}{2}\ddot{C}\xi^2)\,\bar{\psi},\\ \frac{\partial^2\bar{V}}{\partial\xi^2} &= -|\bar{\psi}|^2.\end{aligned}\right\} \tag{24}$$

If we compare the rescaled Schrödinger–Poisson system (24) with the rescaled Vlasov–Poisson one (8), some analogies are apparent. The external, confining field due to the transformation is again of harmonic-oscillator type (quadratic

potential). As previously guessed, no friction appears: the friction term is now replaced by a time-dependent mass $\mu(t) = C^2/A^2$, which, as we shall show later, has the same effect of bringing the particles to rest. Now, the arrow of time is revealed by the presence of some time-dependent coefficients in the equations: it points in the direction of increasing mass.

A final remark on the quantum rescaling is in order here: if one divides the first of (24) by A^2 and comes back to the old time t through (12), the factor $A(t)$ disappears from the rescaled Schrödinger equation (note also that the rescalings of both x and ψ depend only on $C(t)$). Therefore the roles of $C(t)$ and $A(t)$ are totally decoupled: the former determines the structure of the solution in ξ space, while the latter only modifies the time scale. As will be seen later, the choice of $A(t)$ plays an important role in the numerical integration.

As a tentative choice for $C(t)$, we shall take the same expansion law found in the classical case, namely

$$C(t) = (1+\Omega t)^2. \tag{25}$$

Numerical simulations will confirm that the conjectured law (25) is indeed also correct for the quantum expansion.

Before turning to numerical simulations, let us verify whether the classical solution can be consistent with the Schrödinger–Poisson system. In order to do this, we rewrite the system (24), in which $C(t)$ is given by (25) and $A(t) = 1$ (as we have seen, the choice of $A(t)$ does not affect the form of the solution):

$$\left.\begin{aligned} i\frac{\partial\bar{\psi}}{\partial t} &= -\frac{1}{2(1+\Omega t)^4}\frac{\partial^2\bar{\psi}}{\partial\xi^2} + (1+\Omega t)^2(\bar{V}+\Omega^2\xi^2)\,\bar{\psi}, \\ \frac{\partial^2\bar{V}}{\partial\xi^2} &= -|\bar{\psi}|^2. \end{aligned}\right\} \tag{26}$$

Since the squared modulus of the wavefunction is normalized to unity, the classical solution corresponds to $|\bar{\psi}|^2 = 2\Omega^2$ inside the interval $[-1/4\Omega^2, 1/4\Omega^2]$ and to zero outside. Integration of the Poisson equation gives $\bar{V} = -\Omega^2\xi^2$ inside the interval, which exactly cancels the transformation potential. Outside this interval, the potential grows quadratically with ξ, with its slope increasing with time. For large times the overall potential $\bar{V}+\Omega^2\xi^2$ should therefore assume the form of an infinite square well (a subsequent simulation, shown in figure 2, confirms this conjecture).

As is well known, the eigenfunctions of the one-dimensional infinite square well are sinusoidal, with nodes at the boundaries of the well. In order to obtain a rectangular density, as in figure 1, sinusoids of high wavenumber need to be present, and consequently the wave function corresponding to the classical asymptotic solution should be strongly oscillating.

In summary, the classical asymptotic solution can, in principle, be consistent with the Schrödinger–Poisson system: the corresponding quantum solution would be a highly oscillating wave function, and its square modulus would have the rectangular shape plotted in figure 1.

The preceding considerations do not of course prove that the classical solution plays the role of an asymptotic attractor for the quantum problem as well. In order to confirm (or to disprove) such a conjecture, one needs to resort to numerical computations. Our numerical scheme solves the rescaled Schrödinger–Poisson system (24), in which $C(t)$ is given by (25).

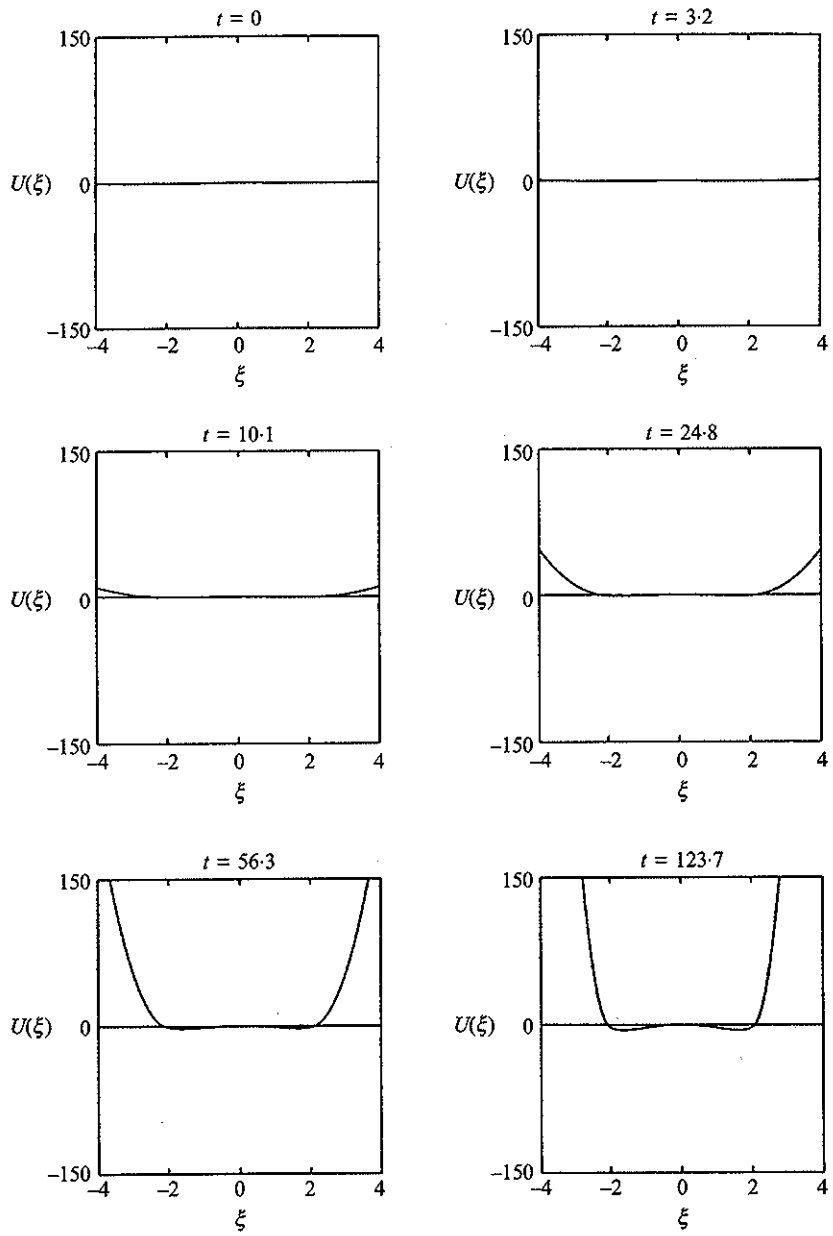

FIGURE 2. Profile of the total potential $U(\xi,t) = (1+\Omega t)^2[\bar{V}(\xi,t)+\Omega^2\xi^2]$ appearing in (26). For large times it approaches the infinite well shape.

The choice of $A(t)$, which determines the time scale, needs to be specified more precisely. The characteristic time τ of our system is given by the inverse of the plasma frequency ω_p:

$$\tau = \omega_p^{-1} = n^{-\frac{1}{2}}, \tag{27}$$

where $n(x,t)$ is the spatial density, which decreases as the inverse of the expansion factor $n \propto (1+\Omega t)^{-2}$. Therefore the characteristic time increases as $1+\Omega t$. In order to keep the ratio between the time-step dt and the characteristic

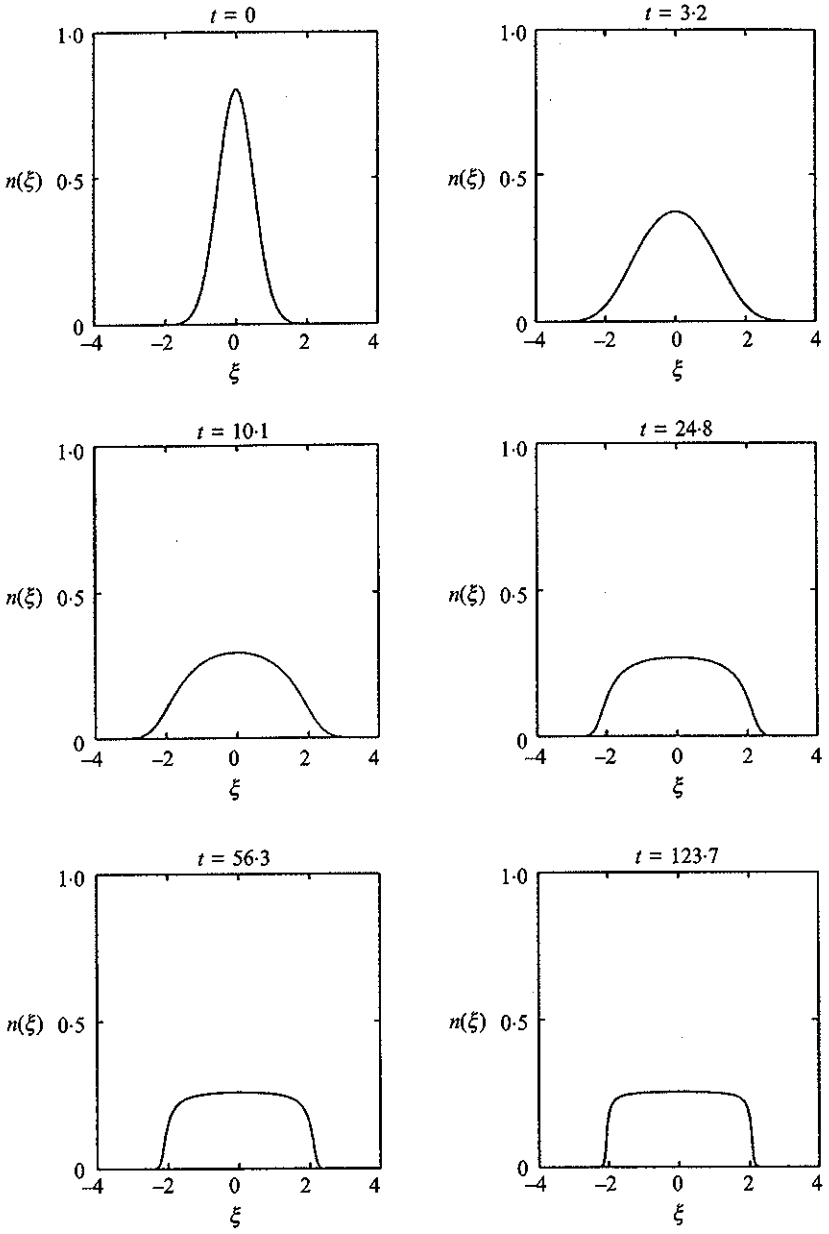

FIGURE 3. Spatial density in the rescaled space, $n(\xi) = |\bar{\psi}(\xi, \vartheta)|^2$. In this simulation we have $\Omega = 2^{-\frac{3}{2}}$; thus the classical profile is a constant in the interval $[-2, 2]$.

time τ constant, one has to choose $A^2(t) = \tau = 1 + \Omega t$, and the relation (6) between t and ϑ becomes

$$1 + \Omega t = e^{\Omega \vartheta}. \tag{28}$$

With this choice, the rescaled Schrödinger equation becomes

$$i\frac{\partial \bar{\psi}}{\partial \vartheta} = -\frac{1}{2e^{3\Omega\vartheta}}\frac{\partial^2 \bar{\psi}}{\partial \xi^2} + e^{3\Omega\vartheta}(\bar{V} + \Omega^2\xi^2)\,\bar{\psi}. \tag{29}$$

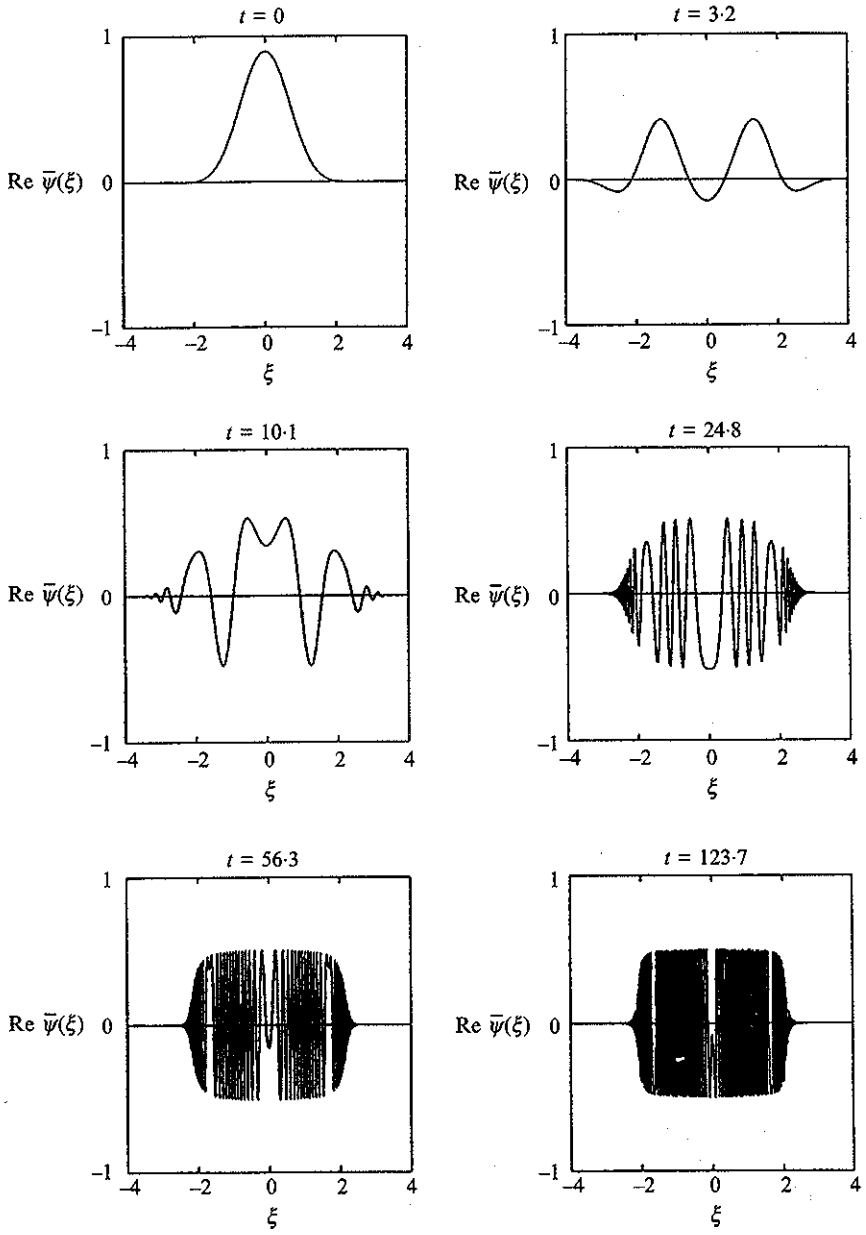

FIGURE 4. Real part of the rescaled wave function $\bar{\psi}(\xi, \vartheta)$ in the same case as figure 3.

This equation has been solved numerically, together with the Poisson equation. A typical result (obtained for $\Omega = 2^{-\frac{3}{2}}$, so that $1/4\Omega^2 = 2$, and for a Gaussian initial condition) is given in figures 3 and 4. The spatial density at different times is plotted in figure 3: its behaviour is exactly that predicted by the classical solution. The real part of the wave function $\bar{\psi}$ (figure 4) is much more complicated, and reveals the presence of high wavenumbers, in accordance with the qualitative explanation given above.

Extensive numerical computation has shown that the rectangular density profile is approached for any initial condition and value of the parameter Ω.

4. The Wigner function

The Wigner transform (Tatarskii 1983) is a useful tool in the study of the classical limit of quantum mechanics. It associates with a wave function $\psi(x)$ a quasi-probability density $W(x,p)$ in phase space, defined by

$$W(x,p) = \frac{1}{2\pi\hbar}\int \psi^*(x-\tfrac{1}{2}\lambda)\,\psi(x+\tfrac{1}{2}\lambda)\exp\left(-i\frac{p\lambda}{\hbar}\right)d\lambda. \tag{30}$$

Although the Wigner function is real, it cannot be regarded as a true probability density, since it almost always assumes negative values. In §5 we shall make extensive use of the Wigner formalism to investigate the classical limit of our expansion problem. It is therefore useful to prove an interesting property connecting the Wigner function to the rescaling transformation.

From (22) we have (the time dependence is understood)

$$\left.\begin{aligned} \psi(x+\tfrac{1}{2}\lambda) &= C^{-\frac{1}{2}}\exp\left[i\frac{\dot{C}}{2C}(x+\tfrac{1}{2}\lambda)^2\right]\bar{\psi}\left(\xi+\frac{\lambda}{2C}\right), \\ \psi^*(x-\tfrac{1}{2}\lambda) &= C^{-\frac{1}{2}}\exp\left[-i\frac{\dot{C}}{2C}(x-\tfrac{1}{2}\lambda)^2\right]\bar{\psi}\left(\xi-\frac{\lambda}{2C}\right). \end{aligned}\right\} \tag{31}$$

We substitute (31) into (30), to give

$$W(x,p) = \frac{1}{2\pi\hbar}\int\frac{1}{C}\bar{\psi}\left(\xi+\frac{\lambda}{2C}\right)\bar{\psi}^*\left(\xi-\frac{\lambda}{2C}\right)\exp\left(-i\frac{\lambda}{C}\frac{pC-\dot{C}x}{\hbar}\right)d\lambda. \tag{32}$$

Defining $\Pi = pC-\dot{C}x$, which corresponds to the classical canonical rescaling (12), and letting $\lambda' = \lambda/C$, we finally obtain

$$W(x,p) = \frac{1}{2\pi\hbar}\int\bar{\psi}\,(\xi+\tfrac{1}{2}\lambda')\,\bar{\psi}^*(\xi-\tfrac{1}{2}\lambda')\exp\left(-i\frac{\lambda'\Pi}{\hbar}\right)d\lambda' \equiv \bar{W}(\xi,\Pi), \tag{33}$$

where we have quite naturally called $\bar{W}$ the Wigner transform of $\bar{\psi}$, according to the definition (30).

The relation (33) shows that the rescaling transformation and the Wigner transform are two commuting operations. In other words, given $\psi(x)$, $\bar{W}(\xi,\Pi)$ can be calculated in two ways: either we first calculate $\bar{\psi}(\xi)$ through (22) and then $\bar{W}$ through (30), or we first look for $W(x,p)$ and then apply the classical rescaling (12) to obtain $\bar{W}$.

The Wigner function obeys the following equation (called the Wigner equation):

$$\frac{\partial W}{\partial t}+\frac{p}{m}\frac{\partial W}{\partial x} = \frac{i}{2\pi\hbar^2}\int\int[V(x-\tfrac{1}{2}\lambda,t)-V(x+\tfrac{1}{2}\lambda,t)]$$

$$\times\exp\left(-i\frac{p-p'}{\hbar}\lambda\right)W(x,p',t)\,dp'\,d\lambda, \tag{34}$$

which, in the limit as $\hbar \to 0$, becomes identical to the classical Vlasov equation. The right-hand side of (34) can be expanded in powers of $\hbar$:

$$\frac{\partial W}{\partial t}+\frac{p}{m}\frac{\partial W}{\partial x}=\frac{\partial V}{\partial x}\frac{\partial W}{\partial p}-\frac{\hbar^2}{24}\frac{\partial^3 V}{\partial x^3}\frac{\partial^3 W}{\partial p^3}+O(\hbar^4), \tag{35}$$

showing that the first correction term is at order $\hbar^2$. Equation (35) also proves that when the potential $V(x,t)$ is a quadratic polynomial in x (possibly time-dependent), the Wigner equation is identical to the Vlasov one, irrespective of the value of Planck's constant.

5. Classical limit

The simulations have produced a partial proof that the quantum electron gas evolves towards a classical solution: although the proof is complete as far as the density is concerned, the complicated structure of the phase of $\bar{\psi}(\xi,\vartheta)$ renders it difficult to pursue the numerical analysis.

Let us therefore come back to the original Schrödinger–Poisson system (1). It can be shown that (1) possesses the following analytical solution (in normalized units):

$$\left.\begin{aligned}\psi(x,t)&=\frac{2^{\frac{1}{2}}}{t}\exp\left(i\frac{x^2}{t}\right),\\ V(x,t)&=-\frac{x^2}{t^2},\quad E=-\frac{\partial V}{\partial x}=\frac{2x}{t^2}.\end{aligned}\right\} \tag{36}$$

It should be noted that the first expression in (36) is a non-normalized wave function. We now want to establish a relation between (36) and the classical asymptotic solution given by (9) and (10). We immediately see that the field is identical to the classical one for $t \to \infty$. In order to compare with (10), let us calculate the Wigner transform of the first expression in (36). The result is

$$W(x,p,t)=\frac{2}{t^2}\delta\left(p-\frac{2x}{t}\right), \tag{37}$$

which is exactly the classical solution (10).

However, since the solution (36) is non-normalized, it cannot represent the asymptotic evolution of a normalized initial condition. Although this might seem in contradiction with the numerical results, which show that an arbitrary initial condition relaxes towards the classical density profile, we believe that the apparent ambiguity can be explained as follows. Both the classical asymptotic solution (10) and the quantum one (36) extend in principle from $x=-\infty$ to $x=+\infty$. However, from a physical point of view, if we start from a normalized initial condition, the solution must remain normalized for any value of t: consequently the distribution function given by (10) needs to be cut off, and set equal to zero outside a certain interval $J \equiv [-L(t), L(t)]$, where $L(t) \propto t^2$, as we have seen in the preceding sections. Formally, this statement implies that the classical solution can be written as

$$W(x,p,t)=\frac{2}{t^2}\delta\left(p-\frac{2x}{t}\right)\Delta(x,t), \tag{38}$$

where $\Delta(x,t)$ is the characteristic function of the interval J:

$$\Delta(x,t) = \begin{cases} 1 & \text{if } x \in J, \\ 0 & \text{elsewhere.} \end{cases} \tag{39}$$

One might be tempted to cut off the quantum solution in the same way, by writing

$$\psi(x,t) = \frac{2^{\frac{1}{2}}}{t} \exp\left(i\frac{x^2}{t}\right)\Delta(x,t), \tag{40}$$

with $\Delta(x,t)$ again given by (39). In fact, this is incorrect, and the reason why is easily understood: in classical mechanics the distribution function may be cut off in the x direction without affecting the momentum distribution; in quantum mechanics cutting the wave function implies modifying both the x and p distributions, so that (40) is no longer a solution of (1). As a matter of fact, the normalization of the wave function only imposes that the *modulus* of Δ has the form given by (39), whereas its phase is not fixed *a priori*. In order to determine the equation that the function Δ must obey, we come back to the rescaling (22), which we write again, with the choice (25) for the factor $C(t)$:

$$\psi(x,t) = \frac{1}{1+\Omega t} \exp\left(i\frac{\Omega x^2}{1+\Omega t}\right)\bar{\psi}(\xi,\vartheta). \tag{41}$$

As $t \to \infty$, (41) becomes

$$\psi(x,t) \sim \frac{1}{t} \exp\left(i\frac{x^2}{t}\right)\bar{\psi}(\xi,\vartheta). \tag{42}$$

Comparison between (42) and (40) is illuminating: the convenient cutting function for the quantum non-normalized solution (36) is nothing other than the rescaled wave function $\bar{\psi}(\xi,\vartheta)$. Indeed, as the numerical simulations have shown, the modulus of $\bar{\psi}$ is actually given by (39). Thus the rescaling automatically treats 'what is classical' in the quantum solution by splitting the solution into two terms: the complex exponential in (40), which represents the classical term, and the rescaled wavefunction $\bar{\psi}$, which gives explicitly the transition from the quantum to the classical regime.

In fact, the approach to the classical limit comes quite naturally from the Schrödinger equation in ξ space, (29), which we rewrite as

$$i\hbar(\vartheta)\frac{\partial\bar{\psi}}{\partial\vartheta} = -\frac{\hbar^2(\vartheta)}{2}\frac{\partial^2\bar{\psi}}{\partial\xi^2} + (\bar{V} + \Omega^2\xi^2)\bar{\psi}, \tag{43}$$

where $\hbar(\vartheta) = e^{-3\Omega\vartheta}$. Formally, (43) represents a system in which Planck's constant depends on time, and tends exponentially to zero.

We recall that (43) was obtained by a rescaling transformation that scales the new time ϑ and space ξ according to the characteristic time and length of the physical system. Although introducing a time-dependent Planck's constant might seem a very formal trick, it is quite surprising that, once time and space are being measured in 'good' units, the classical limit becomes apparent from the very structure of the Schrödinger equation. In a sense, this result indicates that the de Broglie wavelength $\lambda = \hbar/p$ becomes very small with respect to the total length of the system. The interesting aspect of the rescaled equations lies

in the fact that the system they describe keeps its total length approximately constant: therefore in ξ space it is easy to verify that $\lambda \to 0$ with time, both numerically (see figure 4) and analytically, by formally introducing a vanishing Planck's constant in the Schrödinger equation.

In the Wigner formalism the time-dependent Planck's constant trick is even clearer, and will allow us to evaluate the quantum correction terms precisely. From (29) (in which we reintroduce $\hbar$), we can write the Wigner equation for $\bar{W}$, the Wigner transform of $\bar{\psi}$. Following (34), we have

$$\frac{\partial \bar{W}}{\partial \vartheta} + \frac{\Pi}{\mu(\vartheta)} \frac{\partial \bar{W}}{\partial \xi} - 2\mu(\vartheta)\,\Omega^2 \xi \frac{\partial \bar{W}}{\partial \Pi}$$

$$= \frac{i\mu(\vartheta)}{2\pi\hbar^2} \int\int [\bar{V}(\xi - \tfrac{1}{2}\lambda, \vartheta) - \bar{V}(\xi + \tfrac{1}{2}\lambda, \vartheta)] \exp\left[-\frac{i}{\hbar}(\Pi - \Pi')\lambda\right] \bar{W}(\xi, \Pi', \vartheta)\, d\Pi'\, d\lambda, \tag{44}$$

where $\mu(\vartheta) = e^{3\Omega\vartheta}$. The quadratic term $\mu(\vartheta)\,\Omega^2\xi^2$ in the potential is classical, and has therefore been taken out of the integral.

We now want to use the same rescaling as in the classical treatment, which led to the Vlasov–Poisson system (8). In order to do so, we come back to the rescaled velocity η, defined by

$$\eta = \frac{\Pi}{\mu(\vartheta)}, \tag{45}$$

and also rescale the distribution function

$$F(\xi, \eta, \vartheta) = \mu(\vartheta)\, \bar{W}(\xi, \Pi, \vartheta). \tag{46}$$

Introduction of (45) and (46) into (44) yields

$$\frac{\partial F}{\partial \vartheta} + \eta \frac{\partial F}{\partial \xi} - \frac{\partial}{\partial \eta}[(3\Omega\eta + 2\Omega^2\xi) F]$$

$$= \frac{i}{2\pi}\left(\frac{\mu}{\hbar}\right)^2 \int\int [\bar{V}(\xi - \tfrac{1}{2}\lambda, \vartheta) - \bar{V}(\xi + \tfrac{1}{2}\lambda, \vartheta)] \exp\left[-i(\eta - \eta')\frac{\mu}{\hbar}\right] F(\xi, \eta', \vartheta)\, d\eta'\, d\lambda. \tag{47}$$

In deriving (47), we have used the fact that

$$\frac{\partial \bar{W}}{\partial \vartheta} = \frac{\partial}{\partial \vartheta}\left(\frac{F}{\mu}\right) = \frac{1}{\mu}\frac{\partial F}{\partial \vartheta} - \frac{1}{\mu^2}\frac{d\mu}{d\vartheta} F.$$

The time-dependent Planck's constant $\hbar^*(\vartheta) = \hbar/\mu(\vartheta)$ clearly appears in the rescaled Wigner equation (47).

We are now in a position to evaluate the quantum corrections. Expanding the right-hand side of (47) in powers of $\hbar$ (see (35)), we obtain

$$\frac{\partial F}{\partial \vartheta} + \eta \frac{\partial F}{\partial \xi} + \frac{\partial}{\partial \eta}[(\varepsilon - 3\Omega\eta - 2\Omega^2\xi) F] = \frac{1}{24}\left(\frac{\hbar}{\mu}\right)^2 \frac{\partial^2 \varepsilon}{\partial \xi^2} \frac{\partial^3 F}{\partial \eta^3} + O\left[\left(\frac{\hbar}{\mu}\right)^4\right], \tag{48}$$

where $\varepsilon(\xi, \vartheta) = -\partial \bar{V}/\partial \xi$ is the rescaled field, which obeys the Poisson equation

$$\frac{\partial \varepsilon}{\partial \xi} = \int F\, d\eta. \tag{49}$$

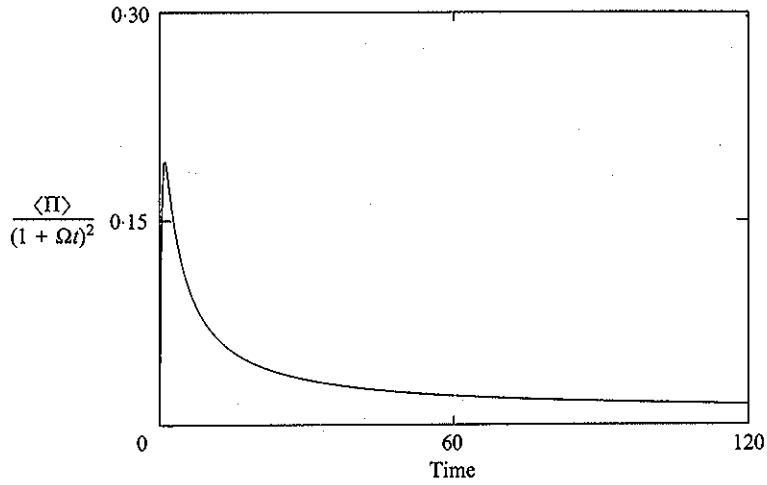

FIGURE 5. Time evolution of the quantity $\langle \Pi \rangle/(1+\Omega t)^2$ as a test for the Ehrenfest's theorem.

From (48) we see that the first quantum correction term goes to zero as $\mu^{-2} = e^{-6\Omega\vartheta} = (1+\Omega t)^{-6}$. This is further proof that in our expansion problem quantum effects rapidly become negligible.

Another way to check numerically whether our system actually tends towards a classical limit is to verify the validity of Ehrenfest's theorem. As is well known, this theorem states that

$$\left.\begin{aligned} \frac{d\langle x \rangle}{dt} &= \langle p \rangle, \\ \frac{d\langle p \rangle}{dt} &= -\left\langle \frac{\partial V}{\partial x} \right\rangle, \end{aligned}\right\} \tag{50}$$

where the angular brackets indicate mean values as usually calculated in quantum mechanics. From the viewpoint of the relations (50), a system shows a classical behaviour whenever

$$\left\langle \frac{\partial V}{\partial x} \right\rangle \approx \left. \frac{\partial V}{\partial x} \right|_{x=\langle x \rangle}.$$

When this relation is satisfied (50) becomes a closed system of differential equations (identical to Newton's laws of motion) for the mean values, which therefore follow the classical trajectories.

For the classical electron gas expansion it is known that $\langle x \rangle \propto t^2$ and $\langle p \rangle \propto t$. In order to see what happens quantum-mechanically, we come back to the rescaling transformation (12), which we rewrite for the mean values:

$$\left.\begin{aligned} \langle x \rangle &= (1+\Omega t)^2 \langle \xi \rangle, \\ \langle p \rangle &= \frac{\langle \Pi \rangle}{(1+\Omega t)^2} + 2\Omega(1+\Omega t)\langle \xi \rangle. \end{aligned}\right\} \tag{51}$$

From the density profile in ξ space (figure 3), it is apparent that $\langle \xi \rangle$ is constant

for large times: consequently the first equation in (51) directly gives the classical relation (in fact, since our initial condition is even, the mean value of ξ calculated from $\xi = -\infty$ to $\xi = +\infty$ is trivially zero; therefore $\langle\ \rangle$ indicates mean values over positive ξ).

The second equation in (51) gives the classical equation if $\langle \Pi \rangle$ does not increase faster than t^2. This conjecture has been verified numerically, and the results are plotted in figure 5: the graph shows the evolution of $\langle \Pi \rangle / (1+\Omega t)^2$ as a function of time: after a transitory period, this quantity approaches a constant value for $t \to \infty$. Thus the first term in the second equation in (51) is negligible compared with the second one, and consequently p grows linearly in t, as expected.

6. Conclusion

In this paper we have investigated the expansion of an electron gas into vacuum, both in the classical and quantum domains. In the latter we have assumed that spin and relativistic effects can be neglected.

The main result of the classical expansion is that all initial conditions evolve asymptotically towards a very simple configuration, given by a uniform density profile, which acts as a universal attractor. This result is obtained by making use of rescaling transformations. In fact, the structure itself of the rescaled equations allows us to guess the form of the asymptotic solution without any further calculation: in order to do this, the presence of a friction term and an external confining potential, both due to the transformation, is a crucial point.

In the quantum domain we first generalize the classical rescaling transformation by imposing the Hamiltonian form of the equations to be conserved. It turns out, in this case, that the classical friction term is replaced by a time-varying mass, which plays the same role of bringing all the particles to rest.

Numerical solution of the rescaled equations proves that the uniform density profile is approached for large times. Analytically, we have shown the existence of a solution of the Schrödinger–Poisson system, the Wigner transform of which gives exactly the classical asymptotic state. In addition, the Wigner formalism has been used to evaluate the quantum correction term to the classical expansion: we have shown that the correction goes to zero as t^{-6}. In fact, since we are dealing with an expanding system with increasing velocities (corresponding to large quantum numbers), the semiclassical result was to be expected. However, we feel that the numerical demonstration is not superfluous, for two reasons.

(i) The quantum solution (36), which is the true counterpart of the classical one (10), is a non-normalized wave function. As shown in §5, the cutting off of the solution is a trivial task for the classical solution, but certainly not for the quantum one. The way in which the uniform density profile is approached is far from obvious.

(ii) All reassuring theorems on the classical limit for large quantum numbers are valid for the *linear* Schrödinger equation. Whether they hold for our *nonlinear* system is an open question, for which numerical simulations suggest a positive answer, at least for this specific model.

In drawing some general conclusions from the preceding discussion, we should stress that quantum plasmas can be a source of very interesting

nonlinear phenomena. It is also a largely unexplored realm. It is our feeling that both numerical and theoretical plasma physicists could bring some fresh ideas into this intriguing domain.

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