PHYSICS OF PLASMAS VOLUME 10, NUMBER 10 OCTOBER 2003

Quantum ion-acoustic waves

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(Received 27 May 2003; accepted 22 July 2003)

The one-dimensional two-species quantum hydrodynamic model is considered in the limit of small mass ratio of the charge carriers. Closure is obtained by adopting an equation of state pertaining to a zero-temperature Fermi gas for the electrons and by disregarding pressure effects for the ions. By an appropriate rescaling of the variables, a nondimensional parameter H, proportional to quantum diffraction effects, is identified. The system is then shown to support linear waves, which in the limit of small H resemble the classical ion-acoustic waves. In the weakly nonlinear limit, the quantum plasma is shown to support waves described by a deformed Korteweg–de Vries equation which depends in a nontrivial way on the quantum parameter H. In the fully nonlinear regime, the system also admits traveling waves which can exhibit periodic patterns. The quasineutral limit of the system is also discussed. [DOI: 10.1063/1.1609446]

I. INTRODUCTION

Quantum transport models have received great attention in recent years mainly due to their relevance for describing quantum effects in plasmas and in microelectronic devices. For quantum plasmas,[1] recent applications include quantum plasma echoes,[2] the expansion of a quantum electron gas into vacuum,[3] quantum plasma instabilities,[4,5,6] the self-consistent dynamics of Fermi gases,[7] and quantum Penrose diagrams.[8] For microelectronics, the ongoing miniaturization process makes classical transport models (e.g., the drift-diffusion model) unable to capture the main physics of a variety of systems such as the resonant tunneling diode and ultra-integrated devices. This motivates the development of quantum transport models for charged particle systems.[9]

Specifically, in this work we focus on the quantum hydrodynamic (QHD) model for plasmas in semiconductors,[7,10–14] The QHD model consists of a set of equations describing the transport of charge, momentum, and energy in a charged particle system interacting through a self-consistent electrostatic potential. The QHD model is constructed in terms of macroscopic variables only, namely, the density and velocity fields, the stress tensor and the electrostatic potential. Mathematically, the QHD model generalizes the fluid model for plasmas, thanks to the inclusion of a quantum correction term, the so-called Bohm potential. This extra term can appropriately describe negative differential resistance in resonant tunneling diodes.[10] Negative differential resistance is based on resonant tunneling, a quantum-driven phenomena which classical transport models cannot take into account. The advantages of the QHD model over kinetic descriptions such as the Wigner–Poisson system[9] are its numerical efficiency,[15,16] the direct use of the macroscopic variables of interest such as momentum and energy, and the easy way the boundary conditions are implemented. The Wigner–Poisson kinetic model, for instance, is a numerically expensive integrodifferential system for which the definition of the boundary conditions is a subtle matter.[17] The weakness of the QHD model, of course, rests in its inability to take into account kinetic effects like Landau damping, driven by resonant wave–particle interaction. Despite the overall simplification, the QHD model can be used, for instance, to describe resonant tunneling diodes,[10,18,19] and, in a modified formulation, ultrasmall high electron mobility transistors.[20] In addition, quantum transport models similar to the QHD model have been used in superfluidity[21] and superconductivity,[22] as well as in the study of metal clusters and nanoparticles, where they are generally referred to as time-dependent Thomas–Fermi (TDTF) models.[23] Finally, hydrodynamic formulations have been employed since the early days of quantum mechanics.[24]

The present work is concerned with two-species quantum plasmas described by the QHD model. Often two-species plasmas are composed of lighter particles (electrons) and more massive particles (ions). This motivates the approximation $m_e/m_i \approx 0$, where m_e and m_i are the masses of electrons and ions, respectively. For classical plasmas, this approximation gives rise to the ion-acoustic mode, whose weakly nonlinear properties are described by the Korteweg–de Vries (KdV) equation. The KdV equation is obtained from a singular expansion in powers of a small parameter proportional to the field amplitude.[25] Classical nonlinear ion-acoustic waves are obtained as traveling-wave solutions for the reduced model in which $m_e/m_i \approx 0$. In the quantum case, the proper framework to analyze ion-acoustic

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waves is provided by the two species QHD model. It is the purpose of this work to analyze this system, following the steps carried out in the case of classical ion-acoustic waves. The relevance of quantum effects for plasmas and semiconductor devices justifies this approach.

The paper is organized as follows. In Sec. II, we present the QHD model for a two species one-dimensional system of charged particles in the electrostatic approximation. Pressure effects are neglected for the more massive ions, whereas the electrons are described by an equation of state appropriate for a zero-temperature Fermi gas. Specifically, our model should be relevant when the following ordering on the temperatures is satisfied:

$$T_{Fi} < T_i < T_e \ll T_{Fe}. \tag{1}$$

Only the electron Fermi temperature is included in our model, while the other three temperature effects are neglected.

Introducing a suitable rescaling of dependent and independent variables, we derive a system of partial differential equations depending on two parameters only, namely H and m_e/m_i. H is a measure of quantum diffraction effects. Taking the limit $m_e/m_i \approx 0$, we obtain a reduced model in which electron inertia is negligible. This reduced model is the main concern of the remaining part of this paper. Linear waves for the reduced model are shown to be described by a dispersion relation which, in the limit of small H, reduces to the dispersion relation for classical ion-acoustic waves (with the ion-acoustic velocity replaced by a quantum ion-acoustic velocity). In Sec. III, we go beyond the linear limit by employing the same singular expansion used for weakly nonlinear classical ion-acoustic waves.[25] These weakly nonlinear quantum ion-acoustic waves are described by a deformed Korteweg–de Vries equation, whose properties are considered in detail. In Sec. IV, the fully nonlinear case is analyzed considering traveling-wave solutions. These solutions satisfy a system of ordinary differential equations not soluble in closed form. However, analysis of the characteristic exponents of the resulting dynamical system indicates the possible existence of periodic patterns confirmed by numerical simulations. In Sec. V, we consider quasineutral solutions, and show that the ions obey a nonlinear Schrödinger equation, with quantum effects appearing at leading order in the mass ratio. Section VI is devoted to the conclusions.

II. REDUCED MODEL AND LINEAR WAVES

We consider a two-species quantum plasma system, composed of electrons and ions. In this situation, the one-dimensional QHD model consists of the continuity and momentum balance equations for both electrons and ions coupled to the Poisson's equation for the self-consistent potential,

$$\frac{\partial n_e}{\partial t} + \frac{\partial(n_e u_e)}{\partial x} = 0, \tag{2}$$

$$\frac{\partial n_i}{\partial t} + \frac{\partial(n_i u_i)}{\partial x} = 0, \tag{3}$$

$$\frac{\partial u_e}{\partial t} + u_e \frac{\partial u_e}{\partial x} = \frac{e}{m_e}\frac{\partial \phi}{\partial x} - \frac{1}{m_e n_e}\frac{\partial p_e}{\partial x} + \frac{\hbar^2}{2m_e^2}\frac{\partial}{\partial x}\left(\frac{\partial^2\sqrt{n_e}/\partial x^2}{\sqrt{n_e}}\right), \tag{4}$$

$$\frac{\partial u_i}{\partial t} + u_i \frac{\partial u_i}{\partial x} = -\frac{e}{m_i}\frac{\partial \phi}{\partial x} + \frac{\hbar^2}{2m_i^2}\frac{\partial}{\partial x}\left(\frac{\partial^2\sqrt{n_i}/\partial x^2}{\sqrt{n_i}}\right), \tag{5}$$

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{e}{\varepsilon_0}(n_e - n_i). \tag{6}$$

Here, $n_e, u_e, m_e, -e$ (resp. n_i, u_i, m_i, e) are the electron (resp. ion) density field, velocity field, mass, and charge, while ε_0 and $\hbar$ are the dielectric and scaled Planck's constants. We are considering a one-dimensional system in the electrostatic approximation with potential ϕ. Finally, $p_e = p_e(n_e)$ is obtained from an equation of state for the electronic fluid. For simplicity, pressure effects are disregarded for ions.

Common choices for p_e are the isobaric (p_e=const), isothermal ($p_e \sim n_e$), and isentropic ($p_e \sim n_e^\gamma$, γ=const $\neq 1$) laws. For definiteness, we assume that the electrons obey the equation of state pertaining to a one-dimensional zero-temperature Fermi gas,[7,26]

$$p_e = \frac{m_e v_{Fe}^2}{3n_0^2} n_e^3. \tag{7}$$

Here, n_0 is the equilibrium density both for electrons and ions, and v_{Fe} is the electronic Fermi velocity, connected to the Fermi temperature T_{Fe} by $m_e v_{Fe}^2/2 = \kappa_B T_{Fe}$, where κ_B is the Boltzmann's constant. The choice of Eq. (7) is not an essential ingredient in what follows, and other equations of state could well be employed. However, Eq. (7) is relevant to the physics of ordinary metals, metal clusters and nanoparticles, for which the electron Fermi temperature is generally much higher than room temperature.

Notice that the model (2)–(7) includes two different quantum effects: (1) quantum diffraction and (2) quantum statistics. Quantum diffraction is taken into account by the terms proportional to $\hbar^2$ in Eqs. (4) and (5). These contributions may be interpreted alternatively as quantum pressure terms or as quantum Bohm potentials. In other applications in semiconductor physics, the Bohm potential is responsible for tunneling and differential resistance effects.[10] The quantum statistics is included in the model via the equation of state [Eq. (7)], which takes into account the fermionic character of the electrons.

The QHD model is a *macroscopic* model, describing the behavior of macroscopic quantities like density and current. For the derivation of the QHD model from a *microscopic* point of view, one can consider a pair of Wigner equations, satisfied by the one-particle Wigner functions for electrons and ions, coupled to the Poisson's equation. The Wigner function plays the same role, in quantum kinetic theory, as the role played by the classical distribution function in classical kinetic theory. In this context, the Wigner equation is the quantum analog of the Vlasov equation describing collisionless classical plasmas. To proceed from kinetic to fluid models, a sensible approach is that of taking moments of the Wigner equation for the two species quantum plasma,[7] exactly in the same way as in gas dynamics or classical plasma physics. Taking the zeroth and first order moments only, we obtain the QHD model with the Bohm potential and a pressure term as shown in Eqs. (2)–(5). Second order moments take into account heat transport, which we disregard here after postulating the equations of state for the electron and ion pressures. These pressure terms provide closure of the transport equations, and are dictated by the statistical properties of the charge carriers. For a pure quantum-mechanical state, the pressure terms are zero: this is in agreement with our understanding of "pressure" as a result of velocity dispersion around the mean velocity of the fluid. The pressure terms chosen here [Eq. (7) for the electrons and zero pressure for the ions] are obtained by neglecting the ion Fermi temperature and assuming a zero-temperature Fermi distribution for the electrons, in the spirit of the ordering shown in Eq. (1). For the electrons, consider the pressure function

$$p_e = m_e\left(\int f_e v^2 dv - n_e u_e^2\right), \tag{8}$$

where $f_e = f_e(x,v,t)$ is the one-particle electron Wigner function, as in Eq. (13) of Ref. 7. Defining a one-dimensional local zero-temperature Fermi distribution for the equilibrium Wigner function $[f_e = n_e(x,t)/(2v_{Fe}(x,t))$ for $|v-u_e(x,t)| < v_{Fe}(x,t); f_e = 0$ otherwise], we obtain

$$p_e = \frac{m_e n_e(x,t) v_{Fe}^2(x,t)}{3}. \tag{9}$$

Here, we allow for a local (nonconstant) Fermi velocity $v_{Fe}(x,t)$. Quantum statistics prevent the collapse of all electrons in a state with velocity $u_e(x,t)$. This is manifested in a nonzero Fermi velocity. In a one-dimensional plasma, the Fermi velocity is linearly dependent on the equilibrium density, $v_{Fe} = \pi\hbar n_0/(2m_e)$. Assuming this linear relation to be valid also for near equilibrium situations, we obtain

$$v_{Fe}(x,t) = \frac{v_{Fe}}{n_0} n_e(x,t). \tag{10}$$

Substituting this last result in Eq. (9), we get the equation of state (7). Notice that the steps in the derivation of this equation of state are all dependent on dimensionality.

In conclusion, the equation of state for electrons was found assuming a local zero-temperature Fermi distribution, a choice dictated by the spin 1/2 statistics for these particles. The Bohm potential, on the other hand, does exist even for a pure quantum-mechanical state, and has nothing to do with the statistical properties of the system. The Bohm potential accounts for such typical quantum effects as tunneling. In a broad sense, we refer to these particularities arising from the wave-like nature of the charge carriers as "quantum diffraction effects." For more details on the mathematical derivation of the QHD model, we refer to Refs. 7 and 10–14.

The ion motion also includes in principle a Bohm potential term. However, in the following, we shall give an argument for neglecting quantum diffraction effects for ions, in view of their large mass.

The electron dynamics can be simplified by using general thermodynamics arguments, since the electrons reach equilibrium faster than the ions due to their smaller mass. In order to show this, let us introduce the following rescaling:

$$\begin{aligned} &\bar{x} = \omega_{pi} x/c_s, \quad \bar{t} = \omega_{pi} t, \\ &\bar{n}_e = n_e/n_0, \quad \bar{n}_i = n_i/n_0, \\ &\bar{u}_e = u_e/c_s, \quad \bar{u}_i = u_i/c_s, \quad \bar{\phi} = e\phi/(2\kappa_B T_{Fe}). \end{aligned} \tag{11}$$

Here, ω_{pe} and ω_{pi} are the corresponding electron and ion plasma frequencies,

$$\omega_{pe} = \left(\frac{n_0 e^2}{m_e \varepsilon_0}\right)^{1/2}, \quad \omega_{pi} = \left(\frac{n_0 e^2}{m_i \varepsilon_0}\right)^{1/2}, \tag{12}$$

whereas n_0 is the equilibrium density. Also, c_s is a quantum ion-acoustic velocity, obtained by replacing the usual electron temperature T_e by $2T_{Fe}$ in the expression for the classical ion-acoustic velocity,

$$c_s = \left(\frac{2\kappa_B T_{Fe}}{m_i}\right)^{1/2}. \tag{13}$$

This definition will be justified later in this work. In addition, we introduce the nondimensional quantum parameter,

$$H = \frac{\hbar \omega_{pe}}{2\kappa_B T_{Fe}}. \tag{14}$$

Note that H^2 is proportional to the r_s parameter of the electron gas, which is the Wigner–Seitz radius in units of the Bohr radius; r_s takes on values in the range 2–6 for metallic electrons.

Using the new variables and dropping bars to simplify the notation, we obtain from Eqs. (4) and (5),

$$\frac{m_e}{m_i}\left(\frac{\partial u_e}{\partial t} + u_e \frac{\partial u_e}{\partial x}\right) = \frac{\partial \phi}{\partial x} - n_e \frac{\partial n_e}{\partial x} + \frac{H^2}{2}\frac{\partial}{\partial x}\left(\frac{\partial^2 \sqrt{n_e}/\partial x^2}{\sqrt{n_e}}\right), \tag{15}$$

$$\frac{\partial u_i}{\partial t} + u_i \frac{\partial u_i}{\partial x} = -\frac{\partial \phi}{\partial x} + \frac{m_e}{m_i}\frac{H^2}{2}\frac{\partial}{\partial x}\left(\frac{\partial^2 \sqrt{n_i}/\partial x^2}{\sqrt{n_i}}\right). \tag{16}$$

The small electron inertia forces the electron fluid to attain equilibrium almost immediately. Hence, neglecting the left-hand side of Eq. (15) due to $m_e/m_i \ll 1$, integrating once and considering (for instance) the boundary conditions $n_e = 1$, $\phi = 0$ at infinity, we obtain

$$\phi = -\frac{1}{2} + \frac{n_e^2}{2} - \frac{H^2}{2\sqrt{n_e}}\frac{\partial^2}{\partial x^2}\sqrt{n_e}. \tag{17}$$

In general an arbitrary irrelevant gauge function of time can be added to the right-hand side of (17), but we will not consider this possibility since it does not affect the electric field. Equation (17) gives the electrostatic potential in terms of the electron density and its derivatives. If quantum diffraction effects are negligible $(H=0)$, the charge density can be obtained from the potential through an algebraic equation. This is very much like in the classical case, where the electron dynamics is often simplified by assuming an exponential law between the electron density and the potential (Boltzmann factor). Here, however, even for $H=0$ there will be no exponential law, since the electron equilibrium is given by a Fermi–Dirac distribution and not by a Maxwell–Boltzmann one. It should be noted that the limit $H\rightarrow 0$ does not represent the classical approximation $\hbar\rightarrow 0$, since $H\sim 1/\hbar$. The limit $H\rightarrow 0$ may be approached in high density regimes and just indicates that quantum diffraction effects are disregarded, although quantum statistical effects (Fermi–Dirac statistics) are still taken into account in the choice of the equation of state, Eq. (7).

In the ion momentum balance equation (16), the quantum diffraction term may also be disregarded due to $m_e/m_i \ll 1$. This may be viewed as a result from the fact that the de Broglie wavelength is inversely proportional to mass. The larger the de Broglie wavelength in comparison with the typical dimensions of the system, the larger are the quantum diffraction effects.

Using the rescaling (11) and discarding terms proportional to m_e/m_i in Eq. (16), the ion conservation of charge and momentum and Poisson's equations become

$$\frac{\partial n_i}{\partial t}+\frac{\partial(n_i u_i)}{\partial x}=0, \tag{18}$$

$$\frac{\partial u_i}{\partial t}+u_i\frac{\partial u_i}{\partial x}=-\frac{\partial \phi}{\partial x}, \tag{19}$$

$$\frac{\partial^2 \phi}{\partial x^2}=n_e-n_i\,. \tag{20}$$

Equations (18)–(20), together with Eq. (17), provide a reduced model of four equations with four unknown quantities, n_i, u_i, n_e, and ϕ. This reduced model is the basic system to be examined in the following. The only remaining free parameter is H, which measures the effects of quantum diffraction. Physically, H is essentially the ratio between the electron plasmon energy and the electron Fermi energy.

After solving the reduced system of equations, the electron fluid velocity field may be obtained from the electron continuity equation,

$$\frac{\partial n_e}{\partial t}+\frac{\partial}{\partial x}(n_e u_e)=0, \tag{21}$$

supplemented by appropriate boundary conditions.

The reduced model (17)–(20) supports linear waves around the homogeneous equilibrium,

$$n_e=n_i=1, \quad u_i=0, \quad \phi=0. \tag{22}$$

For normalized wave frequency ω and wave number k, the dispersion relation for these linear waves is

$$\omega^2=\frac{k^2(1+H^2k^2/4)}{1+k^2(1+H^2k^2/4)}\,. \tag{23}$$

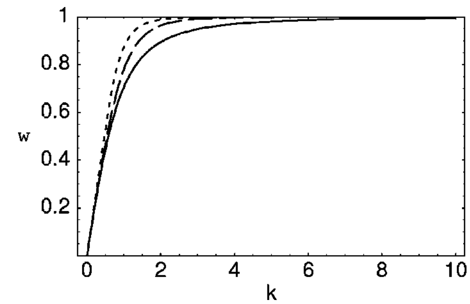

FIG. 1. Normalized dispersion relation for the quantum ion-acoustic mode with $H=0$ (solid line), $H=1.5$ (dashed line), and $H=3$ (dotted line).

For small wave numbers this gives $\omega\simeq k$, or, reintroducing the original physical variables, a wave propagating at the quantum ion-acoustic velocity c_s as given in the definition (13). Equation (23) describes the quantum counterpart of the classical ion-acoustic mode, with a new expression for the acoustic velocity and a correction from quantum diffraction effects. Accordingly, we call this new solution the *quantum ion-acoustic mode*. Like in the case of the classical ion-acoustic waves, this mode describes oscillations of both electrons and ions at low frequency. At the opposite limit of small wavelengths, Eq. (23) gives oscillations at the ion plasma frequency ω_{pi}. (Notice, however, that the QHD model does not apply for small wavelengths.[7]) Figure 1 shows the dispersion relation obtained from Eq. (23) for three different values of the parameter H. Notice that the asymptotic value $\omega=1$ is reached faster the larger are the quantum diffraction effects.

In the following, we investigate the basic properties of the nonlinear solutions for the reduced model (17)–(20).

III. WEAKLY NONLINEAR SOLUTIONS

The reduced model of Eqs. (17)–(20) is the quantum counterpart of the classical reduced model in which the electron dynamics is simplified by assuming that the electronic fluid is at thermodynamic equilibrium. For the classical model one can find coherent structures (solitons). It is therefore relevant to investigate the existence of such coherent structures in the quantum case. We proceed as closely as possible the derivation of weakly nonlinear classical waves for an electron–ion plasma using singular perturbation methods.[25] Introduce the following expansion around the equilibrium:

$$n_i=1+\epsilon\, n_{i1}+\epsilon^2\, n_{i2}+\cdots, \tag{24}$$

$$u_i=\epsilon\, u_{i1}+\epsilon^2\, u_{i2}+\cdots, \tag{25}$$

$$n_e=1+\epsilon\, n_{e1}+\epsilon^2\, n_{e2}+\cdots, \tag{26}$$

where ϵ is a small nonzero parameter proportional to the amplitude of the perturbation. In passing, notice that from Eq. (17) the above expansion implies the following expansion for ϕ:

$$\phi=\epsilon\left(n_{e1}-\frac{H^2}{4}\frac{\partial^2 n_{e1}}{\partial x^2}\right)+\frac{\epsilon^2}{2}\left\{n_{e1}^2+2n_{e2}+\frac{H^2}{2}\left[n_{e1}\frac{\partial^2 n_{e1}}{\partial x^2}-\frac{\partial^2 n_{e2}}{\partial x^2}+\frac{1}{2}\left(\frac{\partial n_{e1}}{\partial x}\right)^2\right]\right\}+\cdots. \quad (27)$$

In addition, we use the following rescaling of space and time variables:

$$\xi=\epsilon^{1/2}(x-t), \quad \tau=\epsilon^{3/2}t. \quad (28)$$

With the new independent coordinates, the perturbation expansion (24)–(26) and the corresponding expansion (27) for the potential, we transform the ion continuity equation (18), the ion momentum balance equation (19), and Poisson's equation (20) into a set of three equations in the form of a power series in ϵ. The resulting system can be written as

$$\frac{\partial}{\partial\xi}(u_{i1}-n_{i1})+\epsilon\left(\frac{\partial n_{i1}}{\partial\tau}+\frac{\partial}{\partial\xi}(-n_{i2}+u_{i2}+n_{i1}u_{i1})\right)=O(\epsilon^2), \quad (29)$$

$$\frac{\partial}{\partial\xi}(n_{e1}-u_{i1})+\epsilon\left[\frac{\partial u_{i1}}{\partial\tau}-\frac{\partial u_{i2}}{\partial\xi}+u_{i1}\frac{\partial u_{i1}}{\partial\xi}-\frac{H^2}{4}\frac{\partial^3 n_{e1}}{\partial\xi^3}+\frac{1}{2}\frac{\partial}{\partial\xi}(n_{e1}^2+2n_{e2})\right]=O(\epsilon^2), \quad (30)$$

$$n_{i1}-n_{e1}+\epsilon\left(n_{i2}-n_{e2}+\frac{\partial^2 n_{e1}}{\partial\xi^2}\right)=O(\epsilon^2). \quad (31)$$

These equations are to be satisfied to all orders in ϵ. The zeroth order terms plus the hypothesis that u_{i1} and n_{i1} vanish as $\xi\to 0$ gives

$$n_{e1}=n_{i1}=u_{i1}\equiv U(\xi,\tau), \quad (32)$$

defining a new function $U(\xi,\tau)$. Equation (32) shows that the mode is quasineutral up to first order.

Taking into account Eq. (32) and the first order terms in Eqs. (29)–(31), there follows

$$\frac{\partial U}{\partial\tau}+\frac{\partial}{\partial\xi}(-n_{i2}+u_{i2}+U^2)=0, \quad (33)$$

$$\frac{\partial U}{\partial\tau}+\frac{\partial}{\partial\xi}\left(-u_{i2}+n_{e2}+U^2-\frac{H^2}{4}\frac{\partial^2 U}{\partial\xi^2}\right)=0, \quad (34)$$

$$\frac{\partial^2 U}{\partial\xi^2}=n_{e2}-n_{i2}. \quad (35)$$

Eliminating n_{e2}, n_{i2}, and u_{i2} from (33)–(35), we obtain a quantum deformation for the Korteweg–de Vries equation,

$$\frac{\partial U}{\partial\tau}+2U\frac{\partial U}{\partial\xi}+\frac{1}{2}\left(1-\frac{H^2}{4}\right)\frac{\partial^3 U}{\partial\xi^3}=0. \quad (36)$$

Quantum diffraction is responsible for the term proportional to H^2. We call Eq. (36) the *deformed Korteweg–de Vries equation* (dKdV).

Notice that the coefficients of the Korteweg–de Vries equation can be arbitrarily fixed through a rescaling of the form $\xi\to a\xi$, $\tau\to b\tau$, $U\to cU$, where a, b, and c are appropriate constants. However, for a fixed choice of units, changing H may affect the nature of the solutions in a fundamental way, as the coefficient of the last term in Eq. (36) is H-dependent. For example, the basic feature of the KdV equation is the balance between dispersion and nonlinearity effects, with as ultimate result the appearance of soliton solutions. This basic property of the KdV equation is destroyed in the dKdV equation in the fine tuning case $H=2$. In this situation, the loss of a dispersive term eventually yields the formation of a shock, as in the case of a one-dimensional force-free ideal and neutral classical fluid.

For $H\neq 2$, soliton solutions still exist, but with a different character for H greater or smaller than 2. For the sake of brevity, we limit ourselves to the one-soliton solution,

$$U(\xi,\tau)=\frac{3c}{2}\operatorname{sech}^2\left(\sqrt{\frac{c}{2}}\frac{(\xi-c\tau)}{(1-H^2/4)^{1/2}}\right), \quad (37)$$

propagating at phase velocity c. Some comments about the solution (37) are in order. First, notice that for $0\leqslant H<2$ the velocity c must be positive. On the other hand, for $H>2$, c ought to be negative, otherwise the soliton solution (37) would be destroyed. Although quantum effects have no influence on the absolute amplitude of the soliton, for H smaller or greater than 2 the soliton exhibits compression or expansion. To see this quantitatively, define s as the distance at which U equals half its maximum absolute amplitude,

$$|U(|\xi-c\tau|=s)|=3|c|/4. \quad (38)$$

The characteristic distance s is a measure of the spreading of the soliton. Solving from Eq. (37), we obtain

$$s\simeq 1.25\left(\frac{1-H^2/4}{c}\right)^{1/2}. \quad (39)$$

For $H<2$ (and $c>0$), quantum effects compress the soliton, as is apparent from Eq. (39). For $H=2$ the soliton collapses, which is in accordance with the nonexistence of the dispersive term in the dKdV equation in this fine tuning case. In the fully quantum case $H>2$ ($c<0$), the soliton starts spreading again as H increases. The ultimate effect of quantum diffraction is the complete smearing out of the soliton. Also notice that in the case $H<2$ we have bright solitons ($U>0$) propagating with a phase velocity $c>0$, whereas in the fully quantum case ($H>2$) we have dark solitons ($U<0$) propagating with a negative phase velocity.

Finally, we remark that for simplicity we have considered only one-soliton solutions for the dKdV equation. Multi-soliton solutions may be easily constructed.

IV. ARBITRARY AMPLITUDE SOLUTIONS

In this section, we investigate the stationary solutions for the system (17)–(20) by assuming all quantities to depend only on the similarity variable,

$$\zeta=x-Mt, \quad (40)$$

where M is a dimensionless constant. For these traveling-wave solutions, Eqs. (18)–(19) give the first integrals

$$J=n_i(u_i-M), \quad (41)$$

$$E=\tfrac{1}{2}(u_i-M)^2+\phi. \quad (42)$$

Eliminating the ion velocity yields

$$n_i = \frac{|J|}{\sqrt{2}(E-\phi)^{1/2}}, \tag{43}$$

which expresses the ion density in terms of the electrostatic potential. Defining

$$n_e \equiv A^2 \tag{44}$$

and using Eqs. (17), (20), and (43), we obtain the system

$$\frac{d^2A}{d\zeta^2} = \frac{A}{H^2}(-1+A^4-2\phi), \tag{45}$$

$$\frac{d^2\phi}{d\zeta^2} = A^2 - \frac{|J|}{\sqrt{2}(E-\phi)^{1/2}}. \tag{46}$$

The formal limit $H=0$ is singular in the sense that in this case Eq. (45) becomes an algebraic equation for A (n_e) in terms of ϕ.

The system (45)–(46) is a pair of second order ordinary differential equations describing the stationary modes of the quantum plasma, depending on the parameters J, E, and H. The structure and nonlinearity feature of this equation, however, prevent any hope for exact solution. Despite this, it is possible to construct an exact conservation law by applying the following reasoning. Let us introduce the (complex) change of variables,

$$\overline{A} = iA, \quad \overline{\phi} = \phi/H, \quad \overline{\zeta} = \zeta/H. \tag{47}$$

In these variables, the system (45)–(46) takes on the Hamiltonian form,

$$\frac{d^2\overline{A}}{d\overline{\zeta}^2} = -\frac{\partial W}{\partial \overline{A}}, \quad \frac{d^2\overline{\phi}}{d\overline{\zeta}^2} = -\frac{\partial W}{\partial \overline{\phi}}, \tag{48}$$

in terms of the pseudopotential $W = W(\overline{A},\overline{\phi})$ given by

$$W = \frac{\overline{A}^2}{2} - \frac{\overline{A}^6}{6} + \sqrt{2}|J|(E - H\overline{\phi})^{1/2} + H\overline{A}^2\overline{\phi}. \tag{49}$$

The last term in Eq. (49) is the only term responsible for the coupling in Eqs. (45)–(46). If that term were missing, we would have a pair of noninteracting nonlinear oscillators.

From the Hamiltonian formulation (48) there follows immediately the energy-like first integral,

$$I = \frac{1}{2}\left(\frac{d\overline{A}}{d\overline{\zeta}}\right)^2 + \frac{1}{2}\left(\frac{d\overline{\phi}}{d\overline{\zeta}}\right)^2 + W(\overline{A},\overline{\phi}), \tag{50}$$

which, expressed in terms of the original variables, gives the exact constant of motion,

$$I = -\frac{H^2}{2}\left(\frac{dA}{d\zeta}\right)^2 + \frac{1}{2}\left(\frac{d\phi}{d\zeta}\right)^2 - \frac{A^2}{2} + \frac{A^6}{6} + \sqrt{2}|J|(E-\phi)^{1/2} - A^2\phi. \tag{51}$$

Unfortunately, the level surfaces of I are never convex, a fact that prevents its use as a Lyapunov function for the stability analysis of the critical points of the system. However, some further insight about the stability of the system can be obtained by linearization around the spatially homogeneous solutions of Eqs. (45)–(46). These equilibria are found by setting the right-hand sides of Eqs. (45)–(46) to zero together with taking $dA/d\zeta = d\phi/d\zeta = 0$. There are two possible homogeneous solutions,

$$A_0 = [E + \tfrac{1}{2} \pm ([E+\tfrac{1}{2}]^2 - J^2)^{1/2}]^{1/4}, \tag{52}$$

$$\phi_0 = \tfrac{1}{2}[E - \tfrac{1}{2} \pm ([E+\tfrac{1}{2}]^2 - J^2)^{1/2}], \tag{53}$$

which we refer to as high and low density equilibria [plus and minus sign in (52)–(53), respectively]. Both equilibria can exist if and only if

$$E + 1/2 \geqslant |J|. \tag{54}$$

Otherwise the homogeneous solutions become complex.

The linear stability regimes can be assessed by assuming

$$A = A_0 + \alpha, \quad \phi = \phi_0 + \beta \tag{55}$$

and retaining only terms up to first order in α and β. By doing this we obtain the following linear system, for low density regimes,

$$\frac{d^2\alpha}{d\zeta^2} = \frac{2A_0}{H^2}(2A_0^3\alpha - \beta), \tag{56}$$

$$\frac{d^2\beta}{d\zeta^2} = 2A_0\alpha - \frac{|J|\beta}{2\sqrt{2}(E-\phi_0)^{3/2}}. \tag{57}$$

We have used expressions (52)–(53) whenever useful for notation. Notice that $E - \phi_0 > 0$ whenever $J \neq 0$ according to Eqs. (53) and (54). Hence, for definiteness we consider the case $J \neq 0$ so that there is no singularity on the right-hand side of Eq. (57). In accordance with Eqs. (52) and (54), a nonzero ionic current J also implies that the low density solution will have necessarily $A_0 \neq 0$.

The linear stability properties of Eqs. (56)–(57) are determined by assuming solutions of the form $\alpha = \alpha_0 \exp(k_c\zeta)$, $\beta = \beta_0 \exp(k_c\zeta)$, for constant α_0, β_0, and k_c. Nontrivial solutions are obtained for characteristic eigenvalues k_c given by

$$k_c^2 = \frac{1}{2A_0^2}[\rho^2 - \sigma \pm ([\rho^2+\sigma]^2 - 4\rho^2)^{1/2}], \tag{58}$$

where we have introduced the following parameters:

$$\rho = \frac{2A_0^3}{H}, \quad \sigma = \frac{A_0^2|J|}{2\sqrt{2}(E-\phi_0)^{3/2}}. \tag{59}$$

Equation (58) shows the existence of four characteristic eigenvalues for the linearized motion around both homogeneous equilibria. There is a large range of possible equilibrium configurations according to the various parameters entering the expression for k_c. We restrict ourselves to consider purely oscillatory motion, which amounts to the determination of the conditions for neutral stability. For neutral stability, by definition all characteristic eigenvalues are purely imaginary, which imposes $k_c^2 \leqslant 0$, with the case $k_c = 0$ corresponding to marginal stability.

Let us first study the limit of small quantum diffraction effects in Eq. (58). For $H \ll 1$, one obtains

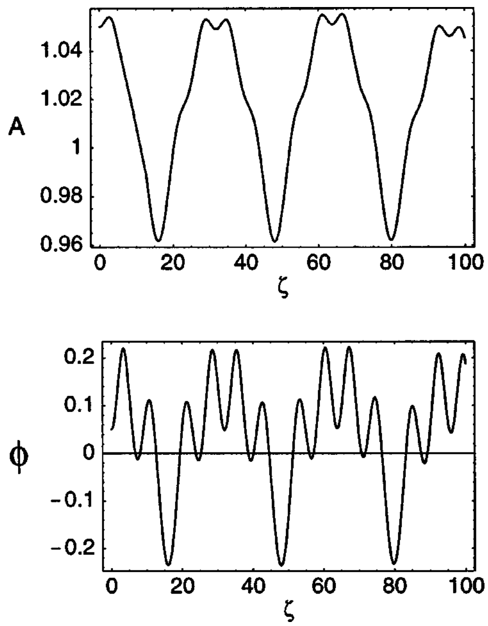

FIG. 2. Numerical solution of Eqs. (45)–(46) with $H=7$, $J=1.22$, and $E=0.744$.

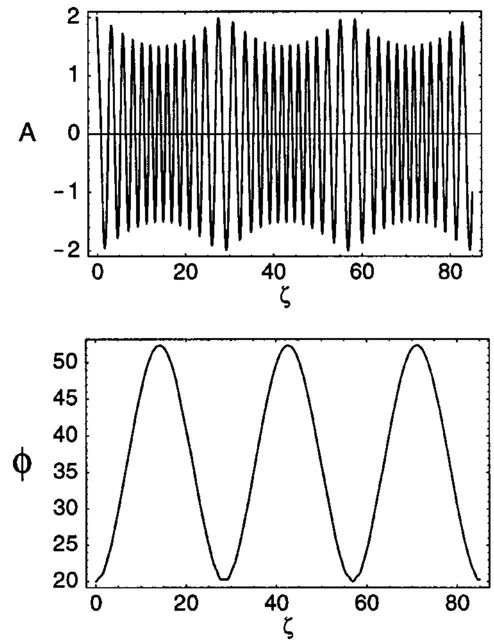

FIG. 3. Numerical solution of Eqs. (45)–(46) with $H=3$, $J=12$, and $E=72$.

$$k_{c+}^2=4A_0^4H^{-2}-A_0^{-2}+O(H^2), \tag{60}$$

$$k_{c-}^2=(1-\sigma)A_0^{-2}+O(H^2). \tag{61}$$

This shows that no oscillatory solutions can exist in the limit $H\rightarrow 0$, as at least one of the eigenmodes (the one with positive sign) possesses a real characteristic eigenvalue. Notice, however, that for H strictly equal to zero, one can reduce Eq. (56) to a purely algebraic equation and substituting the result into Eq. (57). By doing so, only the k_{c-} eigenvalue survives, which does yield oscillatory solutions when $\sigma>1$. In summary, the singular case $H=0$ does support purely oscillatory solutions, but these are destroyed for small, but finite, quantum diffraction effects.

We do not analyze Eq. (58) in its full generality, restricting ourselves to the basic homogeneous equilibrium

$$A_0=1, \quad \phi_0=0. \tag{62}$$

According to Eqs. (52)–(53) and (59), this corresponds to

$$E=J^2/2, \quad \sigma=1/J^2, \quad \rho=2/H. \tag{63}$$

The condition for purely oscillatory solutions (i.e., $k_c^2<0$) yields the inequalities,

$$1<|J|<H/2, \tag{64}$$

which require that $H>2$, in agreement with the previous result that no stable solutions exist for small H.

The oscillations seem to be related to a kind of quantum recurrence, also arising in other quantum plasma phenomena like quantum echoes[2] and quantum two-stream instabilities.[6] Notice that here a space–time recurrence is observed, since the similarity variable $\zeta=x-Mt$ involves both space and time coordinates. Numerical integration of the fully nonlinear system (45)–(46) confirms the existence of such oscillatory motions. Examples of this behavior are given in Figs. 2 and 3. In Fig. 2, the simulation was initialized by assuming that the amplitude A and the potential ϕ were slightly perturbed from the equilibrium (62) at $\zeta=0$, i.e., $A(0)=1+\delta$ and $\phi(0)=\delta$, where $\delta=0.05$. Figure 3 shows the oscillations far from the equilibrium (62); in this case, $A(0)=2$ and $\phi(0)=20$. The singular character of Eq. (47) at $\phi=E$ is manifest in Fig. 4 which shows how A explodes to infinity when $\phi\rightarrow E$. This results from the fact that in this limit, in view of Eq. (42), the ion fluid will move at the wave phase velocity ($u_i\rightarrow M$) an effect that will cause the electrons to accumulate in the wave peaks. [In all the simulations, $(dA/d\zeta)(0)=(d\phi/d\zeta)(0)=0$.]

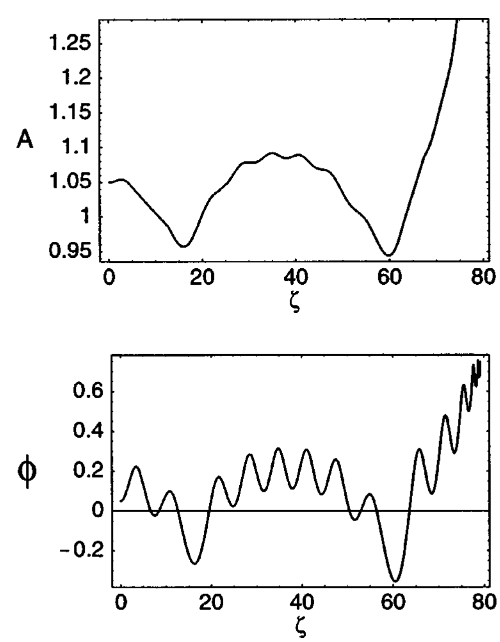

FIG. 4. Numerical solution of Eqs. (45)–(46) with $H=7$, $J=1.23$, and $E=0.756$.

V. QUASINEUTRAL SOLUTIONS

The model used so far to study the propagation of quantum ion-acoustic waves is given by Eqs. (18)–(20), together with Eq. (17). This system can be further simplified by assuming *quasineutrality*, i.e., by neglecting the left-hand side of Poisson's equation (20), which immediately yields $n_i = n_e$. This is accurate when the potential is a slowly varying function of position, i.e., for small wave numbers $k \ll 1$ (in our dimensionless units). One can therefore write n_i instead of n_e in Eq. (17); substitution into the ion momentum conservation equation (19) yields

$$\frac{\partial u_i}{\partial t} + u_i \frac{\partial u_i}{\partial x} = -n_i \frac{\partial n_i}{\partial x} + \frac{H^2}{2} \frac{\partial}{\partial x}\left(\frac{\partial^2 \sqrt{n_i}/\partial x^2}{\sqrt{n_i}} \right). \tag{65}$$

Notice that in Eq. (65) quantum effects (proportional to H^2) appear to zeroth order in the mass ratio, whereas they appeared to first order in Eq. (16).

Equation (65), together with the ion continuity equation (18), form a closed system describing the propagation of quasineutral ion-acoustic waves. Linearizing around the spatially homogeneous equilibrium, as performed in Sec. II, yields the dispersion relation, $\omega^2 = k^2(1 + H^2 k^2/4)$, which should be compared to Eq. (23).

The important feature of this quasineutral regime is that the ion dynamics has a quantum character, even though, because of their large mass, they should behave in a completely classical manner. The reason is that, because of quasineutrality, the ions are instantaneously driven by the electrons, which of course do behave quantum-mechanically. This is an interesting phenomenon: a species that is classical when on its own (the ions), may behave as a quantum fluid when immersed in a bath of particles with quantum properties (the electrons). Notice that quantum effects are relevant for wave numbers satisfying $Hk \geqslant 1$. Combining this inequality with the condition of validity of the quasineutral model $k \ll 1$, yields that H must be large in order to observe significant quantum effects. This condition can be satisfied in metal clusters and nanoparticles.[7,23]

Finally, the above effect can be made even more apparent by rewriting Eqs. (18) and (65) as a single nonlinear Schrödinger equation for the pseudo-wave-function;

$$\Psi_i(x,t) = \sqrt{n_i(x,t)}\, \exp(iS_i(x,t)/H), \tag{66}$$

with S_i defined implicitly according to $u_i = \partial S_i/\partial x$.[7] The resulting equation for Ψ_i is

$$iH \frac{\partial \Psi_i}{\partial t} = -\frac{H^2}{2} \frac{\partial^2 \Psi_i}{\partial x^2} + \frac{1}{2}|\Psi_i|^4 \quad \Psi_i . \tag{67}$$

From this equation, it is obvious that the ions behave as quantum particles in an effective potential of the form $|\Psi_i|^4$.

Notice that a model very similar to Eq. (67) has been used to describe the dynamics of a degenerate gas of neutral Fermi atoms, possibly trapped in an external potential.[27] This equation can also describe the behavior of a Bose–Einstein condensate in one dimension,[28] for which it replaces the usual Gross–Pitaevskii equation. The authors of Ref. 28 also show the existence of an exact soliton solution for Eq. (67), which has the form of a dip in the spatial density.

Given the huge amount of theoretical and experimental work carried out in recent years on Bose–Einstein condensates and ultracold Fermi gases, it would be highly interesting if ions in metal clusters and nanoparticles could, in certain regimes, mimic the behavior of such low-temperature atom gases.

VI. CONCLUSION

In this work we have investigated the role of quantum diffraction in two-species plasmas in which the inertia of one of the species is negligible. The starting point is the QHD model for transport in charged particle systems. For closure, we postulate a pressureless ion fluid and an electron fluid obeying the equation of state for a zero-temperature one-dimensional Fermi gas. After a convenient rescaling and neglecting the inertia of the lighter charge carriers, we have obtained the reduced model of Eqs. (17)–(20). This reduced model has proven to be a valuable and sufficiently simple tool for the examination of linear, weakly nonlinear and fully nonlinear waves.

Several new features of pure quantum origin have appeared. For the linear waves, we have found a dispersion relation that resembles the classical ion-acoustic dispersion relation when $H \to 0$. The parameter H is a measure of quantum diffraction effects, and is proportional to the ratio between the plasmon energy $\hbar\omega_{pe}$ and the Fermi energy $\kappa_B T_{Fe}$. For weakly nonlinear waves, singular perturbation theory gives rise to a deformed KdV equation depending on H. Now three regimes are possible. For $H<2$, we observe a quantum compression of the classical one-soliton solution. For $H=2$, the quantum diffraction exactly matches the classical dispersion term in the KdV equation. Hence, for $H=2$ there is no soliton at all, but only free streaming, eventually producing a shock wave. Finally, for $H>2$ quantum effects smear out the classical one-soliton solution. In the fully nonlinear case, we obtain traveling-wave solutions satisfying the dynamical system (45)–(46). This dynamical system presents strong nonlinearities and does not seem to be soluble in closed form, though it does admit an exact first integral as shown in Sec. IV. The linear stability analysis of its fixed points shows the possible existence of periodic regimes for a restricted range of parameters. Numerical simulations confirm the predictions of linear stability analysis.

Finally, we have considered the special case where the ion–electron plasma is quasineutral. In this regime, valid for long wavelengths, the ion dynamics can be described by a set of two hydrodynamic equations that contain quantum effects to zeroth order in the electron-to-ion mass ratio. Alternatively, the model can be cast in the form of a nonlinear Schrödinger equation, thus making explicit the presence of quantum effects on the ion dynamics. These models closely resemble those used for the description of ultracold neutral atom gases.

ACKNOWLEDGMENTS

Two of us (F.H. and L.G.G.) thank the Brazilian agency Conselho Nacional de Desenvolvimento Científico e Tecnólogico (CNPq) for financial support.

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