Electronic screening in one-component plasmas: Collective-mode structure

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The Golden-Kalman velocity-average approximation scheme for one-component plasmas is generalized to account for electronic screening effects. New formulas are established for the dispersion and damping of the ion-sound and ion-plasma modes at arbitrary coupling.

Studies of the dynamical properties of strongly coupled plasmas have, for the most part, been directed at one-component-plasma (OCP)[1,2] and binary-ionic-mixture[3–6] configurations where the ions are modeled as mobile classical point particles in a neutralizing background of highly degenerate and *rigid* electrons.

The OCP collective-mode structure is substantially modified when the rigidity constraint is relaxed to allow for electronic screening:[7] at wavelengths long compared with the Thomas-Fermi screening distance $\kappa_e^{-1}=(\epsilon_F/6\pi n_e e^2)^{1/2}$, the ion-plasma mode is suppressed in favor of ion-sound modes which propagate when the Fermi energy ϵ_F of the electrons is much larger than the thermal energy $(1/\beta)$ of the ions, viz., $\kappa_e \ll \kappa_i = (4\pi n_i Z^2 e^2 \beta)^{1/2}$. When the ions are modeled as a collection of cold noninteracting particles, the propagation velocity is given by the well-known Bohm-Staver formula[8] $V_0=(V_F/\sqrt{3})(\omega_i/\omega_e)$; ω_i and ω_e are the ion and electron plasma frequencies. When the ions are warm and interacting, a generalized hydrodynamic calculation[9–11] leads to the sound speed[5]

$$V=V_0\left[1+\frac{3}{2Z\epsilon_F}\left[\frac{\partial P_i}{\partial n_i}\right]_\beta\right]^{1/2} \tag{1}$$

which features an *isothermal* compressibility correction.

In this paper, I reformulate the Golden-Kalman (GK) velocity-average approximation (VAA) integral equation [Ref. 2(a)] for the OCP ionic polarizability to take account of electronic screening. I then calculate the dielectric response function and longitudinal mode structure in the $k \ll \kappa_i$, $\omega \lesssim \omega_i=(4\pi n_i Z^2 e^2/m_i)^{1/2}$ wave-number–frequency domains and over a range of ion-ion coupling strengths (characterized by $\gamma_{ii}=\kappa_i^3/(4\pi n_i)$ or by $\Gamma=\beta(Ze)^2/a_i$; $a_i=(3/4\pi n_i)^{1/3}$ spanning the entire fluid regime. My calculations result in new ion-sound formulas [Eqs. (16) below] which are structurally different from the Postogna-Tosi expression (1).

In the present work the extreme degeneracy of the electron gas guarantees that electron-electron correlational effects are negligibly small [viz., $\gamma_{ee}=\kappa_e^3/4\pi n_e \sim(\beta\epsilon_F)^{-3/2}\gamma_{ii} \ll \gamma_{ii}$] even up to $\gamma_{ii}\sim 3200$ typical of the OCP crystal phase.[2(e),2(f)] I further suppose that electron-ion interactions are weak compared with ion-ion interactions. This was a principal assumption of the Ref. 5 calculations leading to Eq. (1) and of the recent Ref. 12 statistical mechanical calculations leading to new dynamical structure functions for two-temperature classical electron-ion plasmas.

The three-stage procedure for calculating the ionic polarizability $\alpha_i(\mathbf{k},\omega)$ begins from the linearized VAA kinetic equation [Ref. 2(a)]

$$i(\omega-\mathbf{k}\cdot\mathbf{v})F_i(\mathbf{k},\mathbf{v},\omega)=\frac{Ze}{m_i}[1+u_i(\mathbf{k},\omega)]\mathbf{E}(\mathbf{k},\omega)\cdot\frac{\partial}{\partial\mathbf{v}}F_i^{(0)}(v) \tag{2}$$

linking the perturbed one-particle-distribution-function response $F_i(\mathbf{k},\mathbf{v},\omega)$ to the total (external+induced) electric field perturbation $\mathbf{E}(\mathbf{k},\omega)$;

$$F_i^{(0)}(v)=n_i(\beta m_i/2\pi)^{3/2}\exp(-\beta m_i v^2/2)$$

is the Maxwellian distribution which characterizes the unperturbed state of the ions. The VAA coupling correction

$$u_i(\mathbf{k},\omega)=-\epsilon(\mathbf{k},\omega)\frac{\kappa_i^2}{k^2}\frac{1}{N_i}\sum_{\mathbf{q}\neq 0,\mathbf{k}}\frac{\mathbf{k}\cdot\mathbf{q}}{q^2}\left[i\omega\int_0^\infty dt e^{i\omega t}S_{iii}(\mathbf{k}-\mathbf{q},t;\mathbf{q},t)+S_{iii}(\mathbf{k}-\mathbf{q},t=0;\mathbf{q},t=0)\right] \tag{3}$$

is expressed entirely in terms of three-point ionic structure functions which are defined in Ref. 6; $\epsilon(\mathbf{k}\omega)=1+\alpha_i(\mathbf{k}\omega)+\alpha_e(\mathbf{k}\omega)$ is the dielectric response function. Consistent with the assumption of the previous paragraph, ion-electron correlations are considered to be negligible in the ionic kinetic equation and are accordingly left out. From (2) and the constitutive relation

$$\int d^3v\, F_i(\mathbf{k},\mathbf{v},\omega)=-\frac{ik}{4\pi Ze}\alpha_i(\mathbf{k},\omega)E(\mathbf{k},\omega)\,, \tag{4}$$

one readily obtains the first-stage expression for the ionic polarizability

$$\alpha_i(\mathbf{k},\omega)=\alpha_{i0}(\mathbf{k},\omega)[1+u_i(\mathbf{k},\omega)]\ , \tag{5}$$

where $\alpha_{i0}(\mathbf{k},\omega)$ is its random-phase approximation (RPA) value.

The second-stage calculation consists in converting (3) into a more tractable nonlinear-response-function expression via the nonlinear fluctuation-dissipation theorem (NLFDT)[13(a),13(b)]

$$\mathrm{Im}\left[\frac{1}{\mu\nu}\frac{\alpha(\mathbf{q},\mu;p,\nu)}{\epsilon(\mathbf{q},\mu)\epsilon(\mathbf{p},\nu)\epsilon(\mathbf{k},\omega)}-\frac{1}{\mu\omega}\frac{\alpha(-\mathbf{k},-\omega;\mathbf{q},\mu)}{\epsilon^*(\mathbf{k},\omega)\epsilon(\mathbf{q},\mu)\epsilon^*(\mathbf{p},\nu)}-\frac{1}{\omega\nu}\frac{\alpha(\mathbf{p},\nu;-\mathbf{k},-\omega)}{\epsilon(\mathbf{p},\nu)\epsilon^*(\mathbf{k},\omega)\epsilon^*(\mathbf{q},\mu)}\right]$$
$$\approx\frac{\pi\beta^2Z^3e^3n_i}{qpk}S_{iii}(\mathbf{q},\mu;p\nu)\quad(\mathbf{k}=\mathbf{p}+\mathbf{q},\ \ \omega=\mu+\nu)\ . \tag{6}$$

The above NLFDT links a single dynamical three-point ionic structure function to total (ionic+electronic) quadratic polarizabilities, e.g., $\alpha(\mathbf{q},\mu;\mathbf{p},\nu)=\alpha_i(\mathbf{q},\mu;\mathbf{p},\nu)+\alpha_e(\mathbf{q},\mu;\mathbf{p},\nu)$, defined through constitutive relations in Refs. 6(a) and 6(b). The S_{iie}, S_{iei}, S_{iee}, etc. structure-function contributions have been deleted because they are entirely comprised of the much weaker ion-electron pair and ternary correlation functions. The $(1/\beta\epsilon_F)^2\ S_{eee}$ contribution is also deleted since $\beta\epsilon_F\gg1$. Substituting (6) into (3) then gives

$$u_i(\mathbf{k},\omega)=i\frac{\kappa_i^2}{k^2}\frac{1}{N_i}\sum_{\mathbf{q}\neq0,\mathbf{k}}\frac{\mathbf{k}\cdot\mathbf{q}}{q^2}\int_{-\infty}^{\infty}d\mu\,\delta_-(\mu)\left[\frac{a(\mathbf{q},\mu;\mathbf{k}-\mathbf{q},\omega-\mu)}{\epsilon(\mathbf{q},\mu)\epsilon(\mathbf{k}-\mathbf{q},\omega-\mu)}+\frac{a(\mathbf{q},\omega-\mu;\mathbf{k}-\mathbf{q},\mu)}{\epsilon(\mathbf{q},\omega-\mu)\epsilon(\mathbf{k}-\mathbf{q},\mu)}\right], \tag{7}$$

where, e.g.,

$$a(\mathbf{q},\mu;\mathbf{k}-\mathbf{q},\omega-\mu)\equiv-\frac{q\,|\,\mathbf{k}-\mathbf{q}\,|\,k}{2\pi\beta^2(Ze)^3n_i}\alpha(\mathbf{q},\mu;\mathbf{k}-\mathbf{q},\omega-\mu)$$

is a conveniently defined reduced quadratic polarizability. The detailed mathematical steps leading to (7) are given in Ref. 2(a). In this extended GK formalism, the responsive electronic background effects modify the ion-ion coupling solely through the $\epsilon\epsilon$-screening clusters [since, e.g., $\epsilon(q,\mu)=1+\alpha_i(\mathbf{q},\mu)+\alpha_e(q,\mu)$]. Equations (5) and (7), when evaluated at high frequency, reproduce through order $1/\omega^4$ the high-frequency sum-rule expansion of $\mathrm{Re}[\alpha_i(\mathbf{k},\omega\to\infty)/\epsilon(\mathbf{k},\omega\to\infty)]$ for arbitrary k and γ values. This is an inherent feature of the GK formalism.[2(a),6(a),6(b)]

In the third-stage development, Eqs. (5) and (7) are made self-consistent at long wavelengths ($k\to0$) by supposing that the quadratic polarizabilities a_i and a_e have RPA-like structures for *arbitrary* values of γ_{ii}. After some algebra [again, see Ref. 2(a) for the details], one arrives at the *dynamical superposition formula*

$$u_i(k\to0,\omega)\simeq\left[\frac{\omega_i}{\omega}\right]^2\left[\frac{k}{\kappa_i}\right]^2\nu(\omega,U_{ii})\ , \tag{8a}$$

$$\nu(\omega,U_{ii})=\frac{4}{15}\frac{\beta U_{ii}}{n_i}-\frac{3}{5N_i}\sum_{\mathbf{q}\neq0,\mathbf{k}}\int_{-\infty}^{\infty}d\mu\,\delta_-(\mu)\frac{\alpha_i(\mathbf{q},\mu)\alpha_i(\mathbf{q},\omega-\mu)}{\epsilon(\mathbf{q},\mu)\epsilon(\mathbf{q},\omega-\mu)}\ . \tag{8b}$$

Elsewhere,[14] it has been rigorously demonstrated that the static ($\omega=0$) limit of the VAA kinetic equation [Ref. 2(a)] generates the entire hierarchy of exact Born-Green-Yvon (BGY) equations for the equilibrium pair, ternary, etc. correlation functions, and the VAA ionic-correlation-energy density therefore can be assumed to be determined from highly accurate Monte Carlo numerical simulations[15] or from an independent theoretical approach. For example, the DeWitt-Rosenfeld calculations provide[16]

$$\frac{\beta U_{ii}(\Gamma)}{n_i}=-0.9\Gamma+0.97\Gamma^{1/4}$$
$$-0.5+1.575\Gamma^{-1/4}-0.042\,56\Gamma^{-1/2}\ ; \tag{9}$$

the first right-hand-side numerical coefficient is very nearly identical to the Madelung constant for the bcc ionic crystal and is indicative of strongly developed order in the liquid phase. At weak coupling ($\gamma_{ii}\ll1$), the correlation-energy density is calculated from the formula

$$\frac{\beta U_{ii}(\gamma_{ii})}{n_i}=-\tfrac{1}{2}\gamma_{ii}\ . \tag{10}$$

Again, observe that at high frequencies $\omega\gg\omega_i$ and Γ arbitrary, the combined Eqs. (5), (8a), and (8b) reproduce the exact (small-k) limit of the crucially important sum-rule coefficient

$$\Omega_i^{(4)}(\mathbf{k})=\int_0^{\infty}\frac{d\omega}{2\pi}\omega^3\mathrm{Im}\frac{\alpha_i(\mathbf{k},\omega)}{\epsilon(\mathbf{k},\omega)}$$
$$=\omega_i^2(\omega_i^2+\omega_e^2)+\omega_i^4\frac{k^2}{\kappa_i^2}\left[3+\frac{4}{15}\frac{\beta U_{ii}}{n_i}\right] \tag{11}$$

of the $1/\omega^4$ term in the expansion of α_i/ϵ. Thus internal consistency between the third-stage development of the approximation scheme and the $\omega\to\infty$ limit of the second-stage VAA expression (7) is guaranteed.

As to the noninteracting electrons, it suffices here to quote the textbook polarizability formula[17]

$$\alpha_e(\mathbf{k},\omega)=\frac{4\pi e^2}{\hbar k^2}\int_{p<p_F} d^3p\frac{2}{(2\pi\hbar)^3}\left[\frac{1}{\omega+(\hbar k^2/2m_e)-\mathbf{k}\cdot\mathbf{v}+i0}-\frac{1}{\omega-(\hbar k^2/2m_e)-\mathbf{k}\cdot\mathbf{v}+i0}\right] \tag{12}$$

describing the linear response of a completely degenerate electron gas. For the frequency range $(\hbar k^2/2m_e)\ll\omega\ll kV_F$ of interest in the present paper, (12) simplifies to

$$\alpha_e(\mathbf{k},\omega)=\frac{6\pi n_e e^2}{\epsilon_F k^2}\left[1+\frac{i\pi}{2}\frac{\omega}{kV_F}\right] . \tag{13}$$

Note that (13) also describes the linear response of relativistic electrons if one stipulates that

$$\epsilon_F=(m_e^2c^4+\hbar^2c^2k_F^2)^{1/2}-m_ec^2 .$$

Equations (5), (8a), (8b), and (13) can now be consolidated into the long-wavelength dispersion relation

$$\epsilon(k\to 0,\omega)=1-\frac{\omega_i^2}{\omega^2}-\frac{\omega_i^4}{\omega^4}\frac{k^2}{\kappa_i^2}[3+\nu(\omega,\Gamma)]+\frac{\kappa_e^2}{k^2}\left[1+\frac{i\pi}{2}\frac{\omega}{kV_F}\right]=0 , \tag{14}$$

which leads to the following dispersion and damping formulas for the ion-sound and ion-plasma modes.

Ion-sound mode.

$$k<\kappa_e<(1/a_i)[\min(\sqrt{3\Gamma},1)] ,$$

$$\omega(k\to 0)=\pm\frac{kV}{(1+k^2/\kappa_e^2)}-\frac{i\pi}{4\sqrt{3}}\frac{k}{\kappa_e}\frac{\omega_i^2}{\omega_e} , \tag{15}$$

where the sound speed

$$V=\begin{cases}V_0\left[1+\frac{3}{2Z}(\beta\epsilon_F)^{-1}\left[3-\frac{17\gamma}{60}\right]\right]^{1/2} & \text{for } \gamma<1 \quad (16a)\\ V_0\left[1+\frac{(\kappa_e a_i)^2}{3\Gamma}[3+\mathrm{Re}\nu(0,\Gamma)]\right]^{1/2} & \text{for } \Gamma\geq 1 \quad (16b)\end{cases}$$

and where

$$(\kappa_e a_i)^2=\begin{cases}(12Z/\pi)^{2/3}r_s & \text{for } p_F\ll m_ec \quad (17a)\\ (81Z^2/2\pi)^{1/3}(e^2/\hbar c) & \text{for } p_F\gg m_ec . \quad (17b)\end{cases}$$

Equations (16a) and (16b) reveal that as Γ increases from zero, V decreases from its maximum RPA value $V(\gamma=0)>V_0$ to the Bohm-Staver sound speed V_0 at $\Gamma=15$ $[\mathrm{Re}\nu(0,15)=-3]$ and then approaches the minimum value

$$V(\Gamma\to\infty)=V_0(1-.08\kappa_e^2a_i^2)^{1/2} .$$

Ion-plasma mode.

$$\kappa_e<k<(1/a_i)[\min(\sqrt{3\Gamma},1)] ,$$

$$\omega(k)\simeq\frac{\omega_i}{(1+\kappa_e^2/k^2)^{1/2}}\left[1+\frac{k^2a_i^2}{3\Gamma}[3+\nu(\omega_i,\Gamma)]\right]^{1/2} . \tag{18}$$

From analytical and numerical calculations in Refs. 2(a) and 2(d)–2(f),

$$\nu(\omega_i,\gamma<1)=-(0.249+i0.056)\gamma ,$$

$$\nu(\omega_i,\Gamma\simeq 8.8)=-(3+i) ,$$

$$\mathrm{Re}\nu(\omega_i,\Gamma\to\infty)=-0.24\Gamma .$$

Equation (18) indicates that the responsive electron background acts to slightly depress the OCP ion-plasma frequency while leaving unaffected the dispersion of the plasma mode.

Formulas (15) and (16) are new while the $\kappa_e=0$ limit of (18) has been extensively studied in Refs. 2. Note the structural difference between the Postogna-Tosi sound speed (1) and its VAA counterparts (16a) and (16b): The former features an isothermal correction which can be valid only if ω tends to zero faster than kV_i; the adiabatic index $c_p/c_v=3$ which shows up in the latter, however, is a consequence of the fact that it is kV_i which tends to zero faster—even at the very low frequencies characteristic of the ion-sound wave. This leads to the conclusion that (1) is derived from an inconsistent set of assumptions. One other important difference should be noted: In the generalized hydrodynamic description[5] of the screened OCP, the ion-sound wave is damped by order-k^2 ion viscous transport; in the present VAA description, however, it is the order-k electron Landau damping which is dominant for $k<\kappa_e$. Note that recent experiments[18] in *equal-temperature* plasmas indicate that the ions are very collisional, so that order-k^2 damping is expected there. However, since those experimental conditions do not satisfy the $\beta\epsilon_F\gg 1$ assumption of the present work, the two very different damping mechanisms are not in conflict.

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