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LETTER TO THE EDITOR

Self-motion and collective behaviour of classical one-component plasmas

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Abstract. The self- and collective motions of one-component plasmas are investigated with the aid of a kinetic theory of classical fluids developed recently by Sjögren and Sjölander. Present calculations show a strong coupling between self- and collective motions and a change in the behaviour of the plasma dispersion relation with increasing density, in agreement with computer simulations.

In recent years molecular dynamics (MD) simulation has been used to study individual particle and collective behaviour of one-component plasmas (OCP) (Hansen *et al* 1975). These calculations have shown two interesting features: (i) the single-particle motion shows a strong coupling to the collective modes, especially at high densities; (ii) the slope of the dispersion curve for the plasma oscillations changes sign from positive to negative with increasing density.

In this work we study the single-particle motion through the velocity autocorrelation function and the collective properties of the system through the dynamical structure factor $S(q, \omega)$. The calculations are based on the kinetic theory of classical fluids recently developed by Sjögren and Sjölander (1977, to be referred to as ss).

The OCP is usually characterised by the dimensionless parameter $\Gamma = (Ze)^2/ak_BT$, where Ze is the ionic charge and $a = (3/4\pi n)^{1/3}$, where n is the number density. The dynamical properties of the OCP are uniquely determined by Γ and the plasma frequency $\omega_p = (4\pi nZ^2e^2/m)^{1/2}$, where m is the ionic mass.

The normalised velocity autocorrelation function $Z(t)$ is defined as

$$Z(t) = \langle \boldsymbol{v}(t) \cdot \boldsymbol{v}(0) \rangle / \langle v^2 \rangle \tag{1}$$

and satisfies the Mori equation

$$\frac{\mathrm{d}}{\mathrm{d}t} Z(t) + \int_0^t \mathrm{d}t' M(t-t') Z(t') = 0 \tag{2}$$

with the corresponding memory function $M(t)$.

The dynamical structure factor $S(q, \omega)$ is the Fourier transform in space and time of the density–density correlation function, denoted here by $G(r, t)$.

From the ss theory we have the following expression for the Fourier–Laplace transform of $G(r, t)$:

$$F(q, z) = \frac{1}{z} S(q) + \frac{F_s(q, z) - z^{-1}}{1 + (z^2/q^2)[(q^2/z)nc(q) - L(q, z)/k_BT](F_s(q, z) - z^{-1})} \tag{3}$$

where $S(q)$ is the static structure factor, $c(q) = (1 - 1/S(q))/n$ is the direct correlation function, F_s is the self part of F, and L is a certain memory function entering in the ss theory. In equation (3) only coupling between the density and the longitudinal current is included. The dynamical structure factor $S(q, \omega)$ is obtained from $F(q, z)$ through the relation

$$S(q, \omega) = \frac{1}{\pi} \operatorname{Re} F(q, z = i\omega). \tag{4}$$

The term L takes into account collisions between the particles that are not included in the conventional mean field theory. Therefore, if we put $L = 0$, the expression in equation (3) reduces to the mean field theory of Kerr (1968) and Singwi *et al* (1970), which in the limit $q \to 0$ and $\Gamma \ll 1$ reproduces the well known Vlasov results for the OCP.

In the expression for $L(q, t)$ in the ss theory a time-dependent effective potential enters and this is equal to the bare potential at $t = 0$ and goes over to $-c(q)k_B T$ for large times. Here, however, we have adopted a time-independent effective potential and assumed it to be equal to the bare potential $v(q) = 4\pi(Ze)^2/q^2$, which is necessary to satisfy the fourth frequency moment of $S(q, \omega)$. We therefore get the following expression for L (see equation (3.34) in ss):

$$L = L_1 + L_2 - L_s \tag{5}$$

where

$$L_1(q, t) = -n \int \frac{d\boldsymbol{q}'}{(2\pi)^3} \{(\hat{\boldsymbol{q}} \cdot \boldsymbol{q}')v(\boldsymbol{q}') + [\hat{\boldsymbol{q}} \cdot (\boldsymbol{q} - \boldsymbol{q}')]v(\boldsymbol{q} - \boldsymbol{q}')\} F(\boldsymbol{q}', t)$$
$$\times F(\boldsymbol{q} - \boldsymbol{q}', t)(1 - nc(\boldsymbol{q}'))c(\boldsymbol{q} - \boldsymbol{q}')[(\boldsymbol{q} - \boldsymbol{q}') \cdot \hat{\boldsymbol{q}}] \tag{6}$$

$$L_2(q, t) = n^2 k_B T q \int \frac{d\boldsymbol{q}'}{(2\pi)^3} (\hat{\boldsymbol{q}} \cdot \boldsymbol{q}')c(\boldsymbol{q}')F(\boldsymbol{q}', t)F(\boldsymbol{q} - \boldsymbol{q}', t)c(\boldsymbol{q}')c(\boldsymbol{q} - \boldsymbol{q}') \tag{7}$$

and

$$L_s(q, t) = -n \int \frac{d\boldsymbol{q}'}{(2\pi)^3} (\hat{\boldsymbol{q}} \cdot \boldsymbol{q}')v(\boldsymbol{q}')F(\boldsymbol{q}', t)F_s(\boldsymbol{q} - \boldsymbol{q}', t)c(\boldsymbol{q}')(\boldsymbol{q}' \cdot \hat{\boldsymbol{q}}). \tag{8}$$

The memory function $M(t)$ of the velocity autocorrelation function is related to L through the equation

$$M(t) = -L(q = 0, t). \tag{9}$$

Equations (5) to (9) yield the following expression for the memory function $M(t)$:

$$M(t) = -\frac{n}{3m} \int \frac{d\boldsymbol{q}}{(2\pi)^3} q^2 v(q)F(q, t)F_s(q, t)c(q). \tag{10}$$

A very similar formula was recently proposed by Gould and Mazenko (1975). The only difference is that in their expression $v(q)$ is replaced by the direct correlation function $-c(q)k_B T$. Using the bare potential $v(q)$ is however, as pointed out above, necessary to satisfy the fourth frequency moment of $S(q, \omega)$.

Equations (3), (6), (7), (8) and (10) have been solved using an iterative procedure. As an initial approximation for $F(q, t)$ we have adopted Lovesey's expression (Lovesey 1971) from viscoelastic theory. For the self part we have used the Gaussian approximation

$$F_s(q, t) = \exp(-q^2 \langle r^2(t) \rangle) \tag{11}$$

starting with an approximate expression for the mean square displacement $\langle r^2(t)\rangle$ that gives the correct limiting behaviour at large and small times. The details of the calculational procedure will be discussed in a forthcoming paper.

Calculations have been done for $\Gamma = 1$ and $\Gamma = 10$. We have taken the values of $S(q)$ from the results of Monte Carlo calculations of Hansen (1973). Self-consistency was achieved after four iterations for $\Gamma = 1$ and six iterations for $\Gamma = 10$.

In figure 1 we compare our results for $Z(t)$ with MD results of Hansen *et al* (1975). Both for $\Gamma = 1$ and $\Gamma = 10$ the agreement is quite satisfactory. We have also calculated the self-diffusion coefficient D_s, using the well known Kubo formula

$$D_s = \frac{1}{3}\int_0^\infty \langle \boldsymbol{v}(t) \cdot \boldsymbol{v}(0)\rangle \, dt. \tag{12}$$

For $\Gamma = 1$ our value differs by 18% and for $\Gamma = 10$ by 17% from that of Hansen *et al*. In table 1 we list the positions of the plasmon peaks at $\Gamma = 1$ and $\Gamma = 10$ obtained from

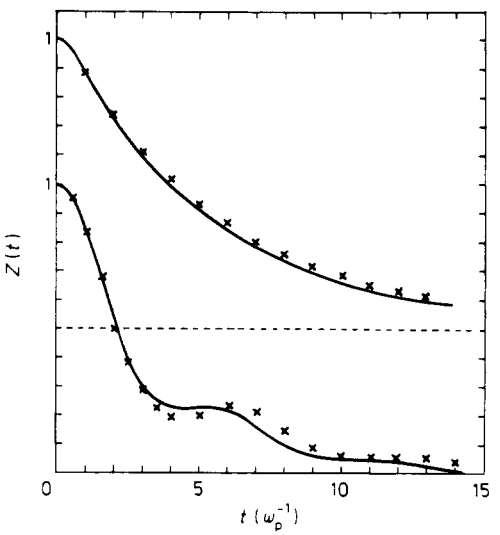

Figure 1. The normalised velocity autocorrelation function $Z(t)$. The full curve is from theory and the crosses are the MD results of Hansen *et al* (1975). The upper results are for $\Gamma = 1$ and the lower results for $\Gamma = 10$.

Table 1. The frequency (in units of ω_p) of the plasmon peak for different values of q (in units of a^{-1}) for $\Gamma = 1$ and $\Gamma = 10$. $\omega(q)_{MD}$ are the corresponding MD results of Hansen *et al* (1975).

$\Gamma = 1$					
q	0·6	0·8	1·0	1·2	1·4
$\omega(q)$	1·05	1·10	1·15	1·35	1·36
$\omega(q)_{MD}$	1·28	1·29	~1·32	~1·34	~1·35
$\Gamma = 10$					
q	1·0	1·3	1·6	1·9	2·25
$\omega(q)$	1·0	0·98	0·90	0·88	0·85
$\omega(q)_{MD}$	0·98	0·97	0·94	~0·91	~0·86

the present calculation together with the MD results. Finally, in figure 2 we present our results for $S(q, \omega)$ for $q = 0{\cdot}6$ and $1{\cdot}4$ Å^{-1} for $\Gamma = 1$ and for $q = 1{\cdot}29$ and $6{\cdot}12$ Å^{-1} for $\Gamma = 10$ together with the MD results.

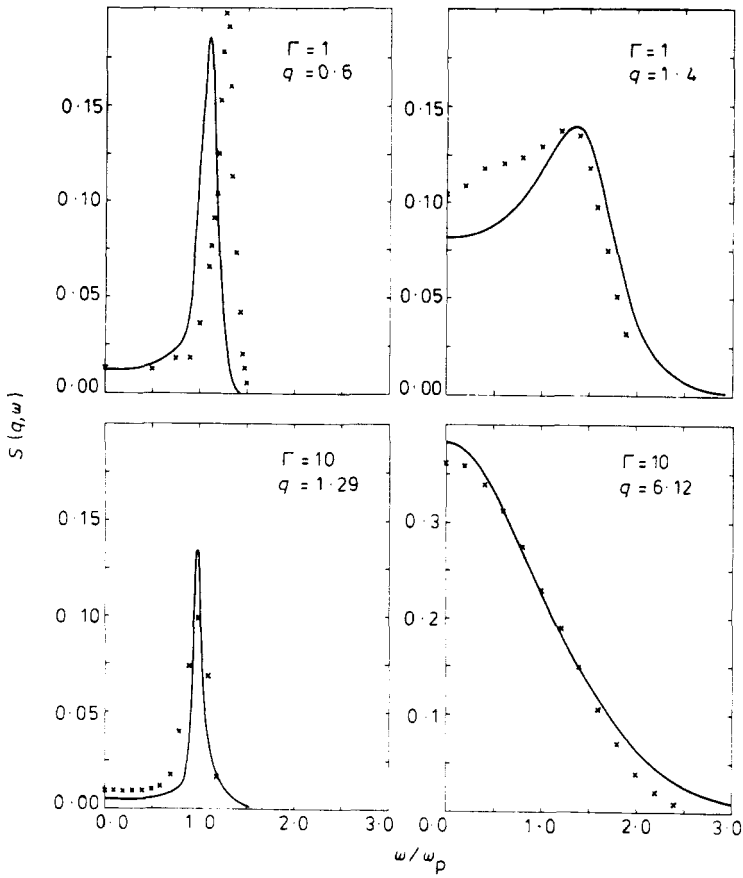

Figure 2. The dynamical structure factor $S(q, \omega)$ in units of ω_p^{-1}. q is in units of a^{-1}. The full curve is from theory and the crosses are the MD results of Hansen *et al* (1975).

We find that the present theory gives quite acceptable agreement, keeping in mind that no adjustable parameters enter. Especially, we notice a change in the velocity autocorrelation function from an exponential decay to an oscillatory behaviour with increasing Γ. The oscillations in the self-motion are due to coupling to the density fluctuations in the system as might be expected from the expression for $M(t)$ (equation (10)). For small densities, where the self-diffusion coefficient D_s is large, this coupling is less important because the single-particle motion then decays in a time short compared to that of a plasma oscillation. For larger densities the coupling becomes more important and manifests itself as damped oscillations in the velocity autocorrelation function.

To second order in q the dispersion relation $\omega(q)$ for the plasma oscillations can be written in the form

$$\omega^2(q) = \omega_p^2(1 + q^2/\Gamma) + \mu q^2 \tag{13}$$

where the first term stems from the mean field part and the remaining part, denoted here by μq^2, comes from L. We notice in table 1 that the slope of the dispersion relation changes sign from positive to negative with increasing Γ. For small Γ the mean field part dominates and gives a Vlasov-type dispersion, but the contribution from L increases with increasing Γ and for $\Gamma > 3$ the dispersion becomes negative.

It is very gratifying to find that the theory of ss satisfactorily explains the essential features of the dynamics of the OCP, although coupling to transverse current and temperature modes are not included. It would be of great interest to test the present theory for considerably larger values of $\Gamma(\sim 100)$, but unfortunately we could not pursue this program because of the large computer time required for this iterative procedure.

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