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1992 J. Phys. A: Math. Gen. 25 6323

(http://iopscience.iop.org/0305-4470/25/23/027)

J. Phys. A: Math. Gen. 25 (1992) 6323–6334. Printed in the UK

On the theory of plasma oscillations in a non-ideal classical plasma

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Received 21 February 1992

Abstract. Using the diagram technique, a high-frequency expansion (with respect to powers $1/\omega^2$) is obtained for polarization operators defining dielectric function of plasma at arbitrary strong interaction between particles. On this basis the spectrum of plasma oscillations for non-ideal classical one- and two-component plasmas is studied. There is a good agreement with the data of molecular dynamic (MD) calculations without using any adjusting parameters. It is shown that the non-Coulombic nature of interaction between particles has a dramatic influence on the description of the spectrum of plasma oscillations in the classical two-component plasma.

1. Introduction

Presently much attention is paid to the theoretical study of plasma oscillation spectrum $\omega(k)$ in non-ideal systems of charged particles (Ichimaru *et al* 1975, Kalman 1978, Baus and Hansen 1980, Ichimaru 1982, Cauble and Boercker 1983, Ichimaru *et al* 1987, Adamjan *et al* 1989). This is explained first of all by intensive study of dynamic structural factors of plasma systems both in real experiments dealing with the scattering of beams of neutrons, electrons or photons (Temperley *et al* 1968, March and Parinello 1982) and in MD calculations for classical systems (Hansen *et al* 1974, 1975, Hansen and McDonald 1978, 1981). The spectrum of plasma oscillations in such experiments is defined by the positions of maxima $\omega_{\max}(k)$ in the dynamical structural factor with a fixed value of wavevector k. Correspondingly, for the theoretical studies most attention was paid to the investigation of the dynamic structure factor of a plasma. Only on this basis was the spectrum of plasma oscillations determined on the assumption that $\omega(k) \simeq \omega_{\max}(k)$. Naturally, it was assumed that the maxima available in the structure factor were expressed fairly well. The measure of it is the relation of semi-width of the maximum with respect to frequency ω and the respective value $\omega_{\max}(k)$.

At the same time, based on a consistent theoretical study of plasma oscillations as collective excitations in plasma, the spectrum $\omega(k)$ must be defined through the poles of 'density–density' Green function or zeros of dielectric function (Kraeft *et al* 1986). Such an approach, well known in the ideal plasma theory (e.g. Silin and Rukhadze 1961), was successfully used in the research of sound oscillation spectra in liquid metal plasma (Belyayev *et al* 1989). According to this approach, the main problem lies in the calculation of the dielectric function of a non-ideal plasma. Although a considerable number of studies have been dedicated to this problem (apart from those already mentioned, see also Carini *et al* 1980, Gorobchenco and Maksimov 1980, Sjorgen and

Hansen 1982), the successful study of the effects of interaction in dielectric function of plasma with arbitrary values of frequencies and wavevectors k still remains one of the major problems of plasma theory.

However, when studying a plasma oscillation spectrum, it is possible to simplify the problem using the following assumptions:

(a) Proximity of spectra $\omega(k)$ to plasma frequency ω_p,

$$\omega_p = \sum_a \frac{4\pi z_a^2 e^2 n_a}{m_a} \tag{1}$$

where $z_a e$ is the charge, m_a is the mass and n_a is the average density of the number of particles of type a.

(b) Presence of small parameters

$$\frac{k\bar{v}}{\omega_p} \ll 1 \qquad \frac{\bar{\nu}}{\omega_p} \ll 1 \tag{2}$$

where $\bar{v}$ and $\bar{\nu}$ are respectively characteristic speed and frequency of collisions for plasma particles. When studying spectrum $\omega(k)$ in weakly non-ideal plasma, conditions (a) and (b) are sufficient for using a high-frequency (with respect to powers of $1/\omega^2$) expansion for the dielectric function of plasma (Silin and Rukhadze 1961, Kraeft *et al* 1986).

This approach was used for the calculation of the dispersion of plasma oscillations in non-ideal one-component (OCP) and two-component (TCP) plasmas with purely Coulombic potentials of interactions between particles (Allahjarov and Trigger 1992). The divergence associated with the impossibility of a purely classical description of the electron–ion structure factor at small distances was eliminated by simulating quantum effects in this factor.

In this paper the expansion with respect to powers of $1/\omega^2$ for dielectric function is used for studying the spectrum $\omega(k)$ in non-ideal classical plasma. For this purpose, using diagram technique methods, the expansion with respect to powers of $1/\omega^2$ was obtained for the polarization operators defining the dielectric function of plasma at arbitrarily strong interaction between particles. The obtained results well agree with the data of MD calculations (Hansen *et al* 1974, 1975, Hansen and McDonald 1978, 1981) without using any adjusting parameters. It is shown that the account of the non-Coulombic nature of interaction between particles in classical TCP considerably influences the description of plasma oscillation spectra.

2. Basic definitions

Let us consider electrically neutral plasma at temperature T (in energy units)

$$\sum_a z_a e n_a = 0. \tag{3}$$

According to the linear response theory (Akhiezer and Peletminskii 1977) the average density of charge in plasma being exposed to a weak electric field is equal in Fourier components

$$\rho(k, \omega) = L^R_{\rho\rho}(k, \omega + i0)\varphi^{(e)}(k, \omega) \tag{4}$$

where $\varphi^{(e)}(k, \omega)$ is the scalar potential of external electric field, $L^{R}_{\rho\rho}(k, z)$ is the 'charge–charge' retarded Green function being analytical in the upper semi-plane of complex $z(\mathrm{Im}\, z > 0)$

$$L^{R}_{\rho\rho}(k, z) = \sum_{ab} z_a z_b e^2 L^{R}_{ab}(k, z) \tag{5}$$

$$L^{R}_{ab}(k, z) = V^{-1} \langle\langle \delta\hat{n}^{a}_{k} | \delta\hat{n}^{b}_{-k} \rangle\rangle_z \tag{6}$$

where $\delta\hat{n}^{a}_{k} = \hat{n}^{a}_{k} - n_a V \delta_{k,0}$, $\hat{n}^{a}_{k}$ is the Fourier component of the operator of the number density for type a particles,

$$\langle\langle \hat{A} | \hat{B} \rangle\rangle_z = -\frac{i}{\hbar} \int_0^\infty dt \exp(izt) \langle [\hat{A}(t), \hat{B}(0)] \rangle \tag{7}$$

where $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$, $\langle \ldots \rangle$ is the averaging with respect to a large canonical ensemble with exact plasma Hamiltonian, $\hat{A}(t)$ is operator $\hat{A}$ in Heisenberg representation, and V is the system volume.

The spacetime behaviour of charge density,

$$\rho(r, t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int \frac{d^3 k}{(2\pi)^3} \rho(k, \omega) \exp(-i\omega t + ikr)$$

taking (4) into account, is fully determined by singularities of Green function $L^{R}_{\rho\rho}(k, z)$ in the lower semi-plane of complex z. Hence to study the spectrum of longitudinal oscillations $\omega(k)$ it is necessary to define poles $\Omega(k)$ of Green function $L^{R}_{\rho\rho}(k, z)$ at $\mathrm{Im}\, z < 0$. Then

$$\omega(k) = \mathrm{Re}\, \Omega(k). \tag{8}$$

Relation (8) holds only at the condition (Silin and Rukhadze 1961, Kraeft *et al* 1986)

$$\gamma(k) = \left| \frac{\mathrm{Im}\, \Omega(k)}{\mathrm{Re}\, \Omega(k)} \right| \ll 1. \tag{9}$$

In turn, the 'charge–charge' dynamic structure factor

$$\begin{aligned} S_{\rho\rho}(k, \omega) &= \sum_{ab} z_a z_b e^2 S_{ab}(k, \omega) \\ S_{ab}(k, \omega) &= V^{-1} \int_{-\infty}^{\infty} dt \exp(i\omega t) \langle \delta\hat{n}^{a}_{k}(t), \delta\hat{n}^{b}_{-k}(0) \rangle \end{aligned} \tag{10}$$

is directly associated with the 'charge–charge' Green function (Akhiezer and Peletminskii 1977)

$$S(k, \omega) = -2\hbar \left\{ 1 - \exp\left(-\frac{\hbar\omega}{T} \right) \right\}^{-1} \mathrm{Im}\, L^{R}_{\rho\rho}(k, \omega + i0). \tag{11}$$

Therefore, taking into account (9), one can state that

$$\omega(k) = \mathrm{Re}\, \Omega(k) \simeq \omega_{\max}(k). \tag{12}$$

Relation (12) is the basis for comparison of theoretical results for oscillation spectrum $\omega(k)$ with experimental and theoretical data for positions of maxima $\omega_{\max}(k)$ of function $S_{\rho\rho}(k, \omega)$.

The most popular approach for determination of the poles of Green function $L^{\mathrm{R}}_{\rho\rho}(k, z)$ for plasma systems is based on the introduction of longitudinal dielectric function $\varepsilon^{l}(k, z)$ describing the screening effects of external field (Silin and Rukhadze 1961, Kraeft *et al* 1986),

$$L^{\mathrm{R}}_{\rho\rho}(k, z) = \frac{k^2}{4\pi}\left(\frac{1}{\varepsilon^{l}(k, z)} - 1\right). \tag{13}$$

It follows directly from (13) that poles $\Omega(k)$ are defined by equation

$$\varepsilon^{l}(k, z) = 0 \tag{14}$$

which is well known in the theory of plasma oscillation. To study function $\varepsilon^{l}(k, z)$ we make use of the diagram technique methods of perturbation theory (Abrikosov *et al* 1965).

3. Diagram representation for longitudinal dielectric function

The retarded Green function $L^{\mathrm{R}}_{\mathrm{ab}}(k, z)$ (6) is the analytical continuation of the respective temperature Green function

$$L^{\mathrm{T}}_{\mathrm{ab}}(k, \mathrm{i}\Omega_n) = V^{-1}\langle\langle \delta\hat{n}^{\mathrm{a}}_{\mathrm{k}} | \delta\hat{n}^{\mathrm{b}}_{-\mathrm{k}} \rangle\rangle_{\mathrm{i}\Omega_n} \tag{15}$$

from a discrete set of points on imaginary axis $\mathrm{i}\Omega_n = 2\pi \mathrm{i} nT$, $n = 0, 1, \ldots$ to the upper semi-plane of complex z. Using the diagram technique of perturbation theory one can easily make sure that function $L^{\mathrm{T}}_{\mathrm{ab}}(k, \mathrm{i}\Omega_n)$ satisfies the system of equations (e.g. Klyuchnikov and Trigger 1976, Bobrov *et al* 1990)

$$L^{\mathrm{T}}_{\mathrm{ab}}(k, \mathrm{i}\Omega_n) = \Pi_{\mathrm{ab}}(k, \mathrm{i}\Omega_n) + \sum_{\mathrm{cd}} \Pi_{\mathrm{ac}}(k, \mathrm{i}\Omega_n) U_{\mathrm{cd}}(k) L^{\mathrm{T}}_{\mathrm{db}}(k, \mathrm{i}\Omega_n) \tag{16}$$

with $U_{\mathrm{ab}}(k)$ being the Fourier component of interaction potential for particles of type a and b, $\Pi_{\mathrm{ab}}(k, \mathrm{i}\Omega_n)$ being the exact polarization operator which is a part of the Green function which is in turn irreducible in the 'k-channel' along the line of interaction.

In the one-component plasma (OCP) case formulae (16) can be written as (Kraeft *et al* 1986)

$$L^{\mathrm{OCP}}_{\mathrm{aa}} = \frac{\Pi^{\mathrm{OCP}}_{\mathrm{aa}}}{\varepsilon^{\mathrm{OCP}}} \qquad \tilde{\varepsilon}^{\mathrm{OCP}} = 1 - U_{\mathrm{aa}} \Pi^{\mathrm{OCP}}_{\mathrm{aa}}. \tag{17}$$

Solution of the set of equations for a two-component plasma (TCP) leads to the following result (Klyuchnikov and Trigger 1990) ($a \neq b$)

$$\begin{aligned} L^{\mathrm{T}}_{\mathrm{aa}} &= \tilde{\varepsilon}^{-1}[\Pi_{\mathrm{aa}} - U_{\mathrm{bb}}(\Pi_{\mathrm{aa}}\Pi_{\mathrm{bb}} - \Pi^2_{\mathrm{ab}})] \\ L^{\mathrm{T}}_{\mathrm{ab}} &= \tilde{\varepsilon}^{-1}[\Pi_{\mathrm{ab}} - U_{\mathrm{ab}}(\Pi_{\mathrm{aa}}\Pi_{\mathrm{bb}} - \Pi^2_{\mathrm{ab}})] \end{aligned} \tag{18}$$

$$\tilde{\varepsilon} = 1 - \sum_{\mathrm{cd}} U_{\mathrm{cd}} \Pi_{\mathrm{cd}} - (U^2_{\mathrm{ei}} - U_{\mathrm{ee}} U_{\mathrm{ii}})(\Pi_{\mathrm{ee}}\Pi_{\mathrm{ii}} - \Pi^2_{\mathrm{ei}}). \tag{19}$$

In a purely Coulombic case, when

$$U_{\mathrm{ab}}(k) = U_{\mathrm{ab}}{}^{\mathrm{c}}(k) = \frac{4\pi z_{\mathrm{a}} z_{\mathrm{b}} e^2}{k^2} \tag{20}$$

the last term in relation (19) turns to zero and the dielectric function $\tilde{\varepsilon}(k, z)$ being the analytical continuation of function $\tilde{\varepsilon}(k, \mathrm{i}\Omega_n)$ (equation (19)) coincides with the longitudinal dielectric function $\varepsilon^l(k, z)$. This also applies to the case of OCP. Using (18), (19) we find

$$\tilde{\varepsilon}^{-1}(k, z) = 1 + \sum_{\mathrm{ab}} U_{\mathrm{ab}}(k) L^{\mathrm{R}}_{\mathrm{ab}}(k, z). \tag{21}$$

According to (13), (18), (19), zeros of function $\varepsilon^l(k, z)$ are determined by zeros of function $\tilde{\varepsilon}(k, z)$. Therefore the dispersion equation (14) for determination of poles $\Omega(k)$ can be represented as

$$\tilde{\varepsilon}(k, z) = 0 \tag{22}$$

for arbitrary form of interaction between particles. With condition (9) satisfied, the dispersion equation for the spectrum of plasma oscillations $\omega(k) = \mathrm{Re}\,\Omega(k)$ can be written as (Silin and Rukhadze 1961)

$$\mathrm{Re}\;\tilde{\varepsilon}(k, \omega + \mathrm{i}0) = 0. \tag{23}$$

In accordance with the discussion in the introduction, we will use high-frequency (with respect to powers of $1/\omega^2$) expansion in the real part of dielectric function $\tilde{\varepsilon}(k, \omega + \mathrm{i}0)$ to solve equation (23). It should be noted that such an approach cannot be used for the calculation of $\mathrm{Im}\,\Omega(k)$ which is defined by means of the value of $\mathrm{Im}\;\tilde{\varepsilon}(k, \omega(k))$ (Silin and Rukhadze 1961). The quantitative and qualitative estimations of the value of $\mathrm{Im}\,\Omega(k)$ may be found in papers by Carini and Kalman (1984) and Brouwer and Schram (1988).

4. High-frequency expansion for polarization operators

By integrating by parts in (6) and (7) for Green function $L^{\mathrm{R}}_{\mathrm{ab}}(k, z)$, it is easy to make sure that

$$L^{\mathrm{R}}_{\mathrm{ab}}(k, z) = \frac{M^{(1)}_{\mathrm{ab}}(k)}{z^2} + \frac{M^{(2)}_{\mathrm{ab}}(k)}{z^4} + \mathrm{O}(z^{-4}) \tag{24}$$

$$M^{(1)}_{\mathrm{ab}}(k) = \frac{1}{\hbar V} \langle [k_\alpha \hat{j}^{\mathrm{a}\alpha}_{\mathrm{k}}, \hat{n}^{\mathrm{b}}_{-\mathrm{k}}] \rangle \tag{25}$$

$$M^{(2)}_{\mathrm{ab}}(k) = \frac{\mathrm{i}}{\hbar V} \langle [k_\alpha \dot{\hat{j}}^{\mathrm{a}\alpha}_{\mathrm{k}}, k_\beta \hat{j}^{\mathrm{b}\beta}_{-\mathrm{k}}] \rangle. \tag{26}$$

Here $\dot{\hat{A}} = \mathrm{i}/\hbar V[\hat{H}, \hat{A}]$, and $\hat{j}^{\mathrm{a}\alpha}_{\mathrm{k}}$ is the current density operator for type a particles. In deriving formulae (24)–(26), it was taken into account that

$$\dot{\hat{n}}^{\mathrm{a}}_{\mathrm{k}} = \mathrm{i} k_\alpha \hat{j}^{\mathrm{a}\alpha}_{\mathrm{k}}. \tag{27}$$

After a simple but cumbersome calculation of commutators in (25) and (26) (similar calculations are described in detail in papers by Adamjan *et al* 1985, Meyer and Tkachenko 1985) we find

$$M^{(1)}_{\mathrm{ab}}(k) = \frac{n_{\mathrm{a}} k^2}{m_{\mathrm{a}}} \delta_{\mathrm{a,b}} \tag{28}$$

$$M_{ab}^{(2)}(k)=\left(\frac{2n_a k^4}{m_a}\langle T_a\rangle+\frac{\hbar^2 n_a k^6}{4m_a^3}\right)\delta_{a,b}+\int\frac{d^3q}{(2\pi)^3}(k_\alpha q_\alpha)^2$$
$$\times\left[\frac{1}{m_a m_b}U_{ab}(q)S_{ab}(q+k)-\frac{1}{m_a m_a}\sum_c U_{ac}(q)S_{cb}(q+k)\delta_{a,b}\right]$$
$$+\frac{n_a n_b}{m_a m_b}k^4 U_{ab}(k). \tag{29}$$

Here $\langle T_a\rangle$ is the exact average kinetic energy corresponding to a single particle of type a, $S_{ab}(q)$ is the static structure factor,

$$S_{ab}(q)=\delta_{a,b}+(n_a n_b)^{1/2}\int d^3r\, \exp(iqr)(g_{ab}(r)-1) \tag{30}$$

$g_{ab}(r)$ is the exact pair correlation function for particles of types a and b. In the classical limit ($\hbar\to 0$), the second term in the square brackets in the right-hand side of equation (29) is absent, and $\langle T_a\rangle=3T/2$.

Substituting (24)–(29) in (18) and (19), we get the expansion with respect to powers of $1/\omega^2$ for polarization operators:

$$\Pi_{ab}(k,\omega+i0)=\frac{\Pi_{ab}^{(1)}(k)}{\omega^2}+\frac{\Pi_{ab}^{(2)}(k)}{\omega^4}+O(\omega^{-4}) \tag{31}$$

$$\Pi_{ab}^{(1)}(k)=\frac{n_a k^2}{m_a}\delta_{a,b} \tag{32}$$

$$\Pi_{ab}^{(2)}(k)=M_{ab}^{(2)}(k)-\frac{n_a n_b}{m_a m_b}k^4 U_{ab}(k). \tag{33}$$

Relations (31)–(33), with account of (19), determine the high-frequency expansion for the dielectric function which can be used for solving the dispersion equation (23).

Let us note that in the purely Coulombic case (20) the expansion with respect to powers of $1/\omega^2$ for the longitudinal dielectric function is as follows:

$$\varepsilon^l(k,\omega+i0)=1-\frac{\omega_p^2}{\omega^2}-\frac{1}{\omega^4}\sum\left\{\frac{2\omega_a^2k^2}{m_a}\langle T_a\rangle+\frac{\hbar^2\omega_a^2k^4}{m_a^2}\right.$$
$$+\sum(n_a n_b)^{1/2}\int_0^\infty dq\, q^2(S_{ab}(q)-\delta_{a,b})$$
$$\left.\times\left[\frac{z_a^2z_b^2e^4}{m_a m_b}\left(\frac{(q^2-k^2)^2}{k^3q}\ln\left|\frac{q+k}{q-k}\right|-\frac{2q^2}{k^2}+6\right)-\frac{8z_a^3z_be^4}{3m_a^2}\right]\right\}+O(\omega^{-4}) \tag{34}$$

where

$$\omega_a=\left(\frac{4\pi z_a^2e^2}{m_a}\right)^{1/2}.$$

5. Spectrum of plasma oscillations in classical OCP

When studying a simulated one-component system of charged particles with compensating background, as a potential of interaction between particles, the Coulombic potential (20) is usually used. Therefore we will use relation (34) for solution of dispersion equation (23).

According to (34), the OCP of dielectric functions with small wavevectors (accurate to k^2) is as follows (Ichimaru and Tange 1974):

$$\varepsilon^l(k,\omega+\mathrm{i}0)=1-\frac{\omega_\mathrm{p}^2}{\omega^2}-\frac{2\omega_\mathrm{p}^2k^2}{\omega^4m_\mathrm{a}}\langle T_\mathrm{a}\rangle\left\{1+\frac{2\langle U_{\mathrm{aa}}\rangle}{15\langle T_\mathrm{a}\rangle}\right\} \tag{35}$$

where

$$\langle U_{\mathrm{aa}}\rangle=\tfrac{1}{2}\int\frac{\mathrm{d}^3q}{(2\pi)^3}\,U^{\mathrm{C}}_{\mathrm{aa}}(q)(S_{\mathrm{aa}}(q)-1)$$

is the exact average potential energy of OCP per one particle. From (35) the accurate limit relations for $\varepsilon^l(k,\omega+\mathrm{i}0)$ for OCP (Bobrov *et al* 1988, 1990) can be obtained

$$\lim_{k\to0}\varepsilon^l(k,\omega+\mathrm{i}0)=1-\frac{\omega_\mathrm{p}^2}{\omega^2}. \tag{36}$$

In its turn, spectrum $\omega(k)$ of plasma oscillations for OCP with small wavevectors according to (23) and (25) is

$$\omega(k)=\omega_\mathrm{p}\left[1+\frac{k^2}{\omega_\mathrm{p}^2m_\mathrm{a}}\langle T_\mathrm{a}\rangle\left\{1+\frac{2\langle U_{\mathrm{aa}}\rangle}{15\langle T_\mathrm{a}\rangle}\right\}\right]. \tag{37}$$

In particular, for a collision-free plasma (Kraeft *et al* 1986)

$$\omega(k)-\omega_\mathrm{p}\simeq\frac{k^2}{\omega_\mathrm{p}m_\mathrm{a}}\langle T_\mathrm{a}\rangle>0. \tag{38}$$

In non-ideal OCP inequality (38) can be violated, i.e. derivative $\partial\omega(k)/\partial k$ can take negative values (Baus and Hansen 1980). In particular, from (37) it directly follows that

$$\frac{m_\mathrm{a}\omega_\mathrm{p}}{\langle T_\mathrm{a}\rangle}\frac{\partial\omega(k)}{\partial k^2}\bigg|_{k\to0}=1+\frac{2\langle U_{\mathrm{aa}}\rangle}{15\langle T_\mathrm{a}\rangle}. \tag{39}$$

To study the sign in the right-hand side of relation (39) for classical OCP one can use the data of MD calculations (Slattery *et al* 1982), according to which for $\Gamma>1$

$$\frac{2\langle U_{\mathrm{aa}}\rangle}{15\langle T_\mathrm{a}\rangle}=\frac{4}{45}(a\Gamma+b\Gamma^{1/4}+c\Gamma^{-1/4}+d) \tag{40}$$

where

$$\Gamma=\left(\frac{z_\mathrm{a}e}{r_\mathrm{a}T}\right)^{1/2}\qquad r_\mathrm{a}=\left(\frac{3}{4\pi n_\mathrm{a}}\right)^{1/3}$$

$$a=-0.897\,774\qquad b=0.950\,43\qquad c=0.189\,56\qquad d=-0.814\,87.$$

As a result, the derivative $\partial\omega(k)/\partial k$ becomes negative at $\Gamma>13.8$.

To study the spectrum $\omega(k)$ of plasma oscillations for classical OCP for arbitrary wavevectors it is necessary, as seen from (34), to determine the static structure factor $S_{\mathrm{aa}}(q)$. For this purpose we will use determination (30) and calculate the pair correlation function in the hypernetted chain (HNC) approximation

$$g_{\mathrm{aa}}(r)=1+h_{\mathrm{aa}}(r)=\exp\left\{h_{\mathrm{aa}}(r)-c_{\mathrm{aa}}(r)-\frac{U_{\mathrm{aa}}(r)}{T}\right\} \tag{41}$$

taking account of the Ornstein–Zernike relation

$$h_{\mathrm{aa}}(r)=c_{\mathrm{aa}}(r)+n_\mathrm{a}\int\mathrm{d}r_1\,c_{\mathrm{aa}}(r-r_1)h_{\mathrm{aa}}(r_1). \tag{42}$$

The results of calculations in HNC approximation agree well with the data of MD calculations (Ichimaru 1982). The set of equations (41) and (42) is solved within the frames of iteration procedure described in detail in paper by Ng (1974).

The results of calculation of spectrum $\omega(k)$ of plasma oscillations for classical OCP are presented in figure 1, where quantity a is equal to r_a. The obtained results agree well with the data of MD calculations (Hansen *et al* 1974, 1975).

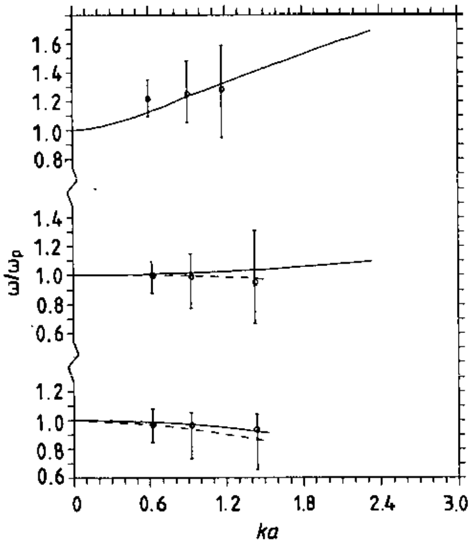

Figure 1. Dispersion curves $\omega(k)$ for OCP. Continuous curves (from top to bottom of figure): calculations for $\Gamma=0.993$, 9.7, 110.4. Broken curves: results of Carini and Kalman (1984) for corresponding Γ. ○: MD data (Hansen *et al* 1974, 1975).

6. Spectrum of plasma oscillations in classical TCP

Spectrum $\omega(k)$ of plasma oscillations in TCP sufficiently differs as compared with the OCP case. First of all, the relation (36) fails to be fulfilled. According to (34) dielectric function in a purely Coulombic case with small wavevectors (accurate to k^2) is

$$\varepsilon^l(k, \omega+\mathrm{i}0) = 1 - \frac{\omega_p^2}{\omega^2} - \frac{\omega_p^4}{\omega^4}\left(1+\frac{z_i m_e}{m_i}\right)^2 (g_{ei}(0)-1)$$
$$- \frac{1}{\omega^4}\sum_a \left\{\frac{2\omega_a^2 k^2}{m_a}\langle T_a\rangle + \sum_b (n_a n_b)^{1/2}\frac{16}{15}\frac{z_a^2 z_b^2 e^4 k^2}{m_a m_b}\int_0^\infty \mathrm{d}q(S_{ab}(q)-\delta_{a,b})\right\}$$
$$+\mathrm{O}(\omega^{-4}). \tag{43}$$

So the spectrum $\omega(k)$ of plasma oscillation in TCP at $k\to 0$ can be either more or less than the plasma frequency ω_p depending on the system parameters. The derivative $\partial\omega(k)/\partial k$ at $k\to 0$ can be negative as in the OCP case.

The second important circumstance is associated with the fact that no purely Coulombic model can be used to describe a classical TCP (as distinct from OCP) due to instability with respect to electron-ion interaction. This circumstance appears first in the calculation of correlation functions, in particular $g_{ab}(r)$ and $S_{ab}(k)$.

This problem is usually solved with the use of efficient interaction potentials accounting for quantum effects at small distances (Kraeft *et al* 1986). In particular, in

MD calculations use is usually made of the following effective potentials (Hansen and McDonald 1978, 1981):

$$U_{ab}(k)=\frac{4\pi z_a z_b e^2}{k^2(1+k^2\lambda_{ab}^2)}. \tag{44}$$

Here

$$\lambda_{ab}^2=\frac{\hbar^2}{2\pi T\mu_{ab}} \qquad \text{and} \qquad \mu_{ab}^{-1}=m_a^{-1}+m_b^{-1}.$$

In r-space, potentials U_{ab} (44) are

$$U_{ab}(r)=\frac{z_a z_b e^2}{r}\left(1-\exp\left(-\frac{r}{\lambda_{ab}}\right)\right). \tag{45}$$

To calculate static structural factors $S_{ab}(q)$ we will use definition (30) and pair distribution functions in the HNC approximation for multi-component systems (Ichimaru *et al* 1987)

$$g_{ab}(r)=\delta_{a,b}+h_{ab}(r)=\exp\left\{h_{ab}(r)-c_{ab}(r)-\frac{U_{ab}(r)}{T}\right\} \tag{46}$$

$$h_{ab}(r)=c_{ab}(r)+\sum_d n_d\int dr_1\, c_{ad}(r-r_1)h_{db}(r_1). \tag{47}$$

Next, assuming that the account of the non-Coulombic nature of interaction is sufficient only for calculation of structural factors $S_{ab}(q)$, we will use for determination of spectra $\omega(k)$ of plasma oscillations in hydrogen TCP the relation (34) for longitudinal dielectric function corresponding to the Coulombic case. The calculation results presented in figure 2 differ qualitatively from the data obtained by MD calculations. Here, the dimensionless length parameter r_s is defined by the ratio of ion–sphere radius to the Bohr radius a_0, i.e.

$$r_s=\frac{a}{a_0}=\frac{am_e e^2}{\hbar^2}.$$

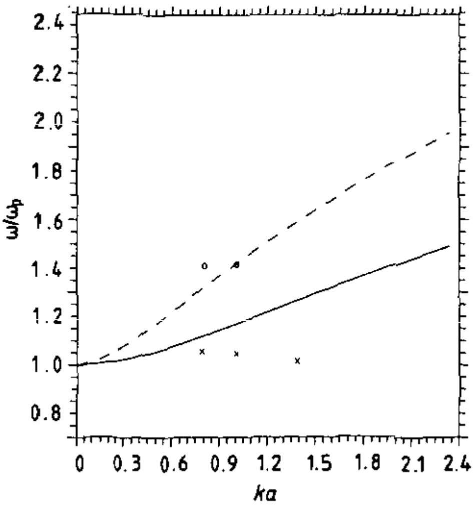

Figure 2. Dispersion curves $\omega(k)$ for TCP using (34). Continuous curve: calculation for parameters $\Gamma=2$, $r_s=1$. Broken curve: calculation for parameters $\Gamma=0.5$, $r_s=1$ and $\Gamma=0.5$, $r_s=0.4$. ×: MD data for $\Gamma=2$, $r_s=1$. ○: MD data for $\Gamma=0.5$, $r_s=1$ (Hansen *et al* 1978, 1981).

The reason is the necessity of a successful account of the non-Coulombic nature of interaction between particles for the calculation of dielectric function in classical TCP. Then, to solve the dispersion equation (23), it is necessary to use determination (19) and high-frequency expansion (31)–(33) for polarization operators Π_{ab}.

When using effective potentials (44), the polarization operators for classical TCP can be conveniently represented as follows:

$$\Pi_{ee}(k,\omega+i0)=\frac{k^2}{4\pi e^2}\left\{\frac{\omega_e^2}{\omega^2}+\frac{k^2\omega_e^4}{\Gamma z_i\omega^4}+\frac{4\omega_e^4}{9\pi\omega^4}[z_i^{-1}A_{ee}(k)+z_i^{-1/2}B_{ei}]\right\}+O(\omega^{-4}) \qquad (48)$$

$$\Pi_{ii}(k,\omega+i0)=\frac{k^2}{4\pi e^2}\left\{\frac{m\omega_e^2}{z_i\omega^2}+\frac{m^2k^2\omega_e^4}{\Gamma z_i\omega^4}+\frac{4m^2\omega_e^4}{9\pi z_i^2\omega^4}[z_i^2A_{ii}(k)+z_i^{3/2}B_{ei}]\right\}+O(\omega^{-4}) \qquad (49)$$

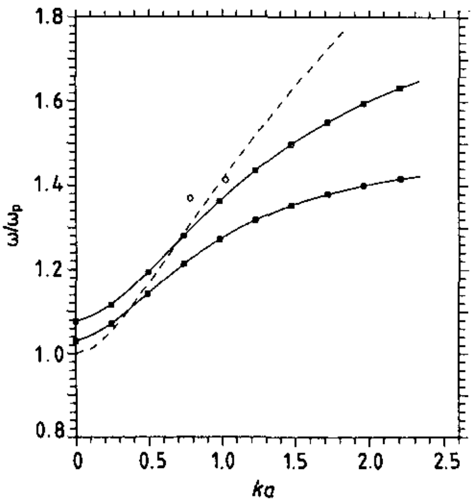

Figure 3. Dispersion curves $\omega(k)$ for TCP. Calculation for parameters $\Gamma=0.5$, $r_s=1$ (□) and $\Gamma=0.5$, $r_s=0.4$ (■). ○: MD data for $\Gamma=0.5$, $r_s=1$ (Hansen *et al* 1978, 1981). The broken curve corresponds to the continuous curve in figure 2, using (34) for parameters $\Gamma=2$, $r_s=1$.

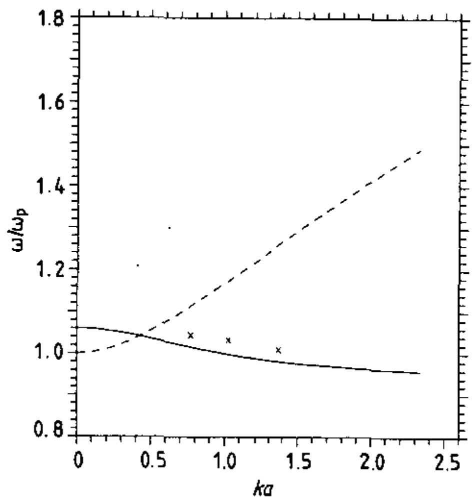

Figure 4. Dispersion curve $\omega(k)$ for TCP. Calculation for parameters $\Gamma=2$, $r_s=1$ (continuous curve). ×: MD data (Hansen *et al* 1978, 1981). The broken curve corresponds to the continuous curve in figure 2, using (34) for parameters $\Gamma=2$, $r_s=1$.

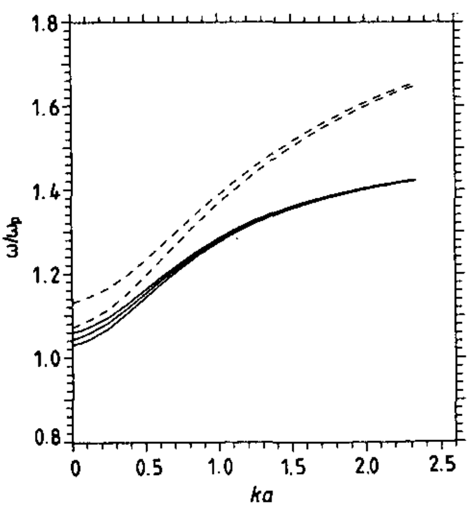

Figure 5. Dispersion curves $\omega(k)$ for TCP at various values of ion charge. Continuous curve: calculation for parameters $\Gamma=0.5$, $r_s=0.4$ (moving up: $z_i=1, 2, 3$). Broken curve: calculation for parameters $\Gamma=0.5$, $r_s=1$ ($z_i=1, 2$).

$$\Pi_{ei}(k,\omega+i0)=-\frac{k^2}{4\pi e^2}\frac{4m\omega_e^4}{9\pi z_i^{1/2}\omega^4}A_{ei}(k)+O(\omega^{-4}) \tag{50}$$

where

$$\Gamma=\frac{e^2}{Tr_i} \qquad \text{and} \qquad m=\frac{m_e}{m_i}$$

$$\begin{aligned}A_{ab}(k)=\int_0^\infty \mathrm{d}q\, q^2(S_{ab}(q)-\delta_{a,b})\left\{\frac{3\tau_{ab}^2}{8k^2}+\frac{3(q^2-k^2)^2}{16qk^3}\ln\left|\frac{q+k}{q-k}\right|\right.\\ \left.-\frac{3(q^2+\tau_{ab}^2-k^2)^2}{32qk^3}\ln\left|\frac{(q+k)^2+\tau_{ab}^2}{(q-k)^2+\tau_{ab}^2}\right|-\frac{\tau_{ab}^2}{2(\tau_{ab}^2+q^2)}\delta_{a,b}\right\}\end{aligned} \tag{51}$$

$$B_{ei}=\int_0^\infty \mathrm{d}q\, q^2 S_{ei}(q)\frac{\tau_{ei}^2}{2(\tau_{ei}^2+q^2)} \tag{52}$$

where

$$\tau_{ab}=r_i/\lambda_{ab}$$

and wavevectors k and q in the relations are made dimensionless with reference to the average distance r_i.

The results of the respective calculations presented in figures 3 and 4 agree well with the data of MD calculations (Hansen and McDonald 1978, 1981). So a successful account of the non-Coulombic nature of interaction between particles has an essential influence on the description of plasma oscillation spectrum of classical TCP.

Figure 5 shows the results of the calculated spectrum $\omega(k)$ for classical TCP for different charges of ions z_i in the assumption that $m_i \sim z_i$.

In conclusion let us stress once again that no adjustment parameters have been used in the calculations. So the use of high-frequency (with respect to powers of $1/\omega^2$) expansion for dielectric function must also be very efficient in studying spectra of plasma oscillations in real plasma systems.

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