



**INTERNATIONAL CENTRE FOR
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PSEUDOCCLASSICAL APPROACH TO ELECTRON AND ION DENSITY CORRELATIONS

IN SIMPLE LIQUID METALS

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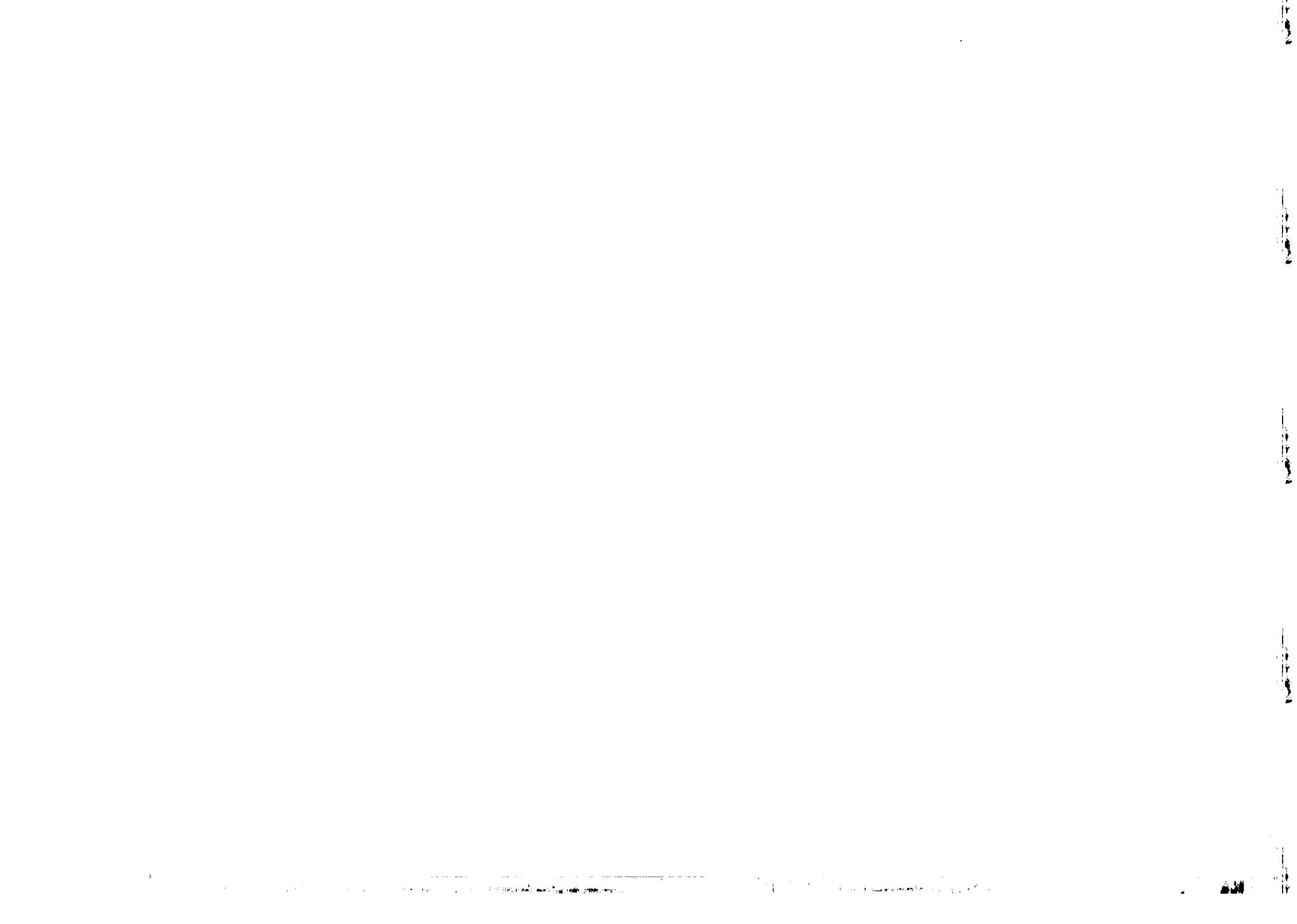
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ABSTRACT

Electron-electron and electron-ion structural correlations in simple liquid metals are treated by using effective pair potentials to incorporate quantal effects into a pseudoclassical description of the electron fluid. An effective pair potential between simultaneous electron density fluctuations is first constructed from known properties of the degenerate jellium model, which are the plasmon sum rule, the Kimball-Niklasson relation and Yasuhara's values of the electron pair distribution function at contact. An analytic expression is thereby obtained in the Debye-Hückel approximation for the electronic structure factor in jellium over a range of density appropriate to metals, with results which compare favourably with those of fully quantal evaluations. A simple pseudoclassical model is then set up for a liquid metal: this involves a model of charged hard spheres for the ion-ion potential and an empty core model for the electron-ion potential, the Coulombic tails being scaled as required by the relation between the long-wavelength partial structure factors and the isothermal compressibility of the metal. The model is solved analytically by a pseudoclassical linear response treatment of the electron-ion coupling and numerical results are reported for partial structure factors in liquid sodium and liquid beryllium. Contact is made for the latter system with data on the electron-electron structure factor in the crystal from inelastic X-ray scattering experiments of Eisenberger, Marra and Brown.

1. INTRODUCTION

Following pioneering work of Cowan and Kirkwood¹⁾ on the structure of an assembly of ionized atoms, there has been continued interest in treating the structure of pure liquid metals as that of two-component fluids of ions and electrons. A number of calculations have been reported for the partial structure factors of such an electron-ion mixture²⁾⁻⁵⁾ and more recently for the ion-ion structure factor of liquid alkali metals from an electron-ion plasma viewpoint⁶⁾⁻⁸⁾. Attention has been drawn to the electron-electron structure factor by measurements of this function from inelastic X-ray scattering experiments on crystalline beryllium and on graphite^{9),10)}.

We approach in this work the evaluation of partial structure factors in simple liquid metals by a method which has been extensively used in the study of dense multicomponent plasmas¹¹⁾. The method involves the construction of effective pair potentials which keep account of quantal effects to some extent, for use in a description of the quantal system by classical statistical mechanics either in a context of liquid-structure integral equations or by computer simulation techniques. One of our aims is to examine whether such a simple approach can yield useful structural information on electron-ion plasmas at temperatures much below the electron degeneracy temperature.

We start in Sec. 2 by constructing an effective pair potential between simultaneous electron density fluctuations in degenerate jellium. The form and the parameters of the effective potential are chosen so that (i) some known structural properties of the electron fluid at long wavelengths and at short distances can be incorporated into the theory and (ii) an analytic form for the pseudoclassical structure factor can be obtained in a range of density appropriate to metals. Comparison of the results with those of quantal evaluations on the degenerate electron fluid¹²⁾⁻¹⁴⁾ is also presented in this section.

An effective electron-ion system is then constructed in Sec. 3. The exact relation which exists between the long-wavelength partial structure factors of the liquid metal and its isothermal compressibility²⁾⁻⁴⁾ is used to relate the strengths of the long-range Coulombic tails in the effective pair potentials. A description of the ionic cores in terms of charged hard spheres for the ion-ion interactions and of empty cores for the electron-ion interactions provides then the simplest realization of the model, which can be solved analytically by appropriate approximations. Numerical results for

partial structure factors in liquid sodium and beryllium are reported in Sec. 4 and compared with available data and theoretical results. Sec. 5 concludes the paper with a summary and discussion.

2. PSEUDOCCLASSICAL MODEL FOR ELECTRON LIQUID STRUCTURE

A marked qualitative similarity has been noticed recently¹⁵⁾ between the electron pair distribution function $g(r)$ in the degenerate electron fluid at large values of the coupling parameter r_s ($r_s \sim 100$) and the pair function in the classical one-component plasma at a suitably chosen coupling strength Γ . As usual these coupling strengths are defined as $r_s = a/a_0$ and $\Gamma = e^2/ak_B T$, where $a = (4\pi n/3)^{-1/3}$ in terms of the electron density n and a_0 is the Bohr radius. A precise correspondence between r_s and the coupling strength of a classical equivalent is indicated by the long wavelength limit of the structure factor $S(k)$. In the degenerate electron fluid this follows from the f-sum rule as

$$\lim_{k \rightarrow 0} S(k) = \frac{1}{2} k \omega_p^2 / 4\pi n e^2, \quad (2.1)$$

ω_p being the electron plasma frequency, whereas classically

$$\lim_{k \rightarrow 0} S(k) = k_s^2 / 4\pi n e^2. \quad (2.2)$$

Evidently from these equations an equivalent classical plasma has a temperature determined by the zero point energy of the plasma excitation, i.e. the long range Coulombic tail of the effective electron-electron potential corresponds to a classical coupling strength given by

$$\Gamma = (4 r_s / 3)^{1/2}. \quad (2.3)$$

This equivalence at large r_s maps fairly accurately the pair functions of the degenerate and classical fluid into each other¹⁵⁾.

In extending the above correspondence between quantal and classical plasma to the range of relatively low coupling strength r_s which is appropriate for electrons in metals ($2 \lesssim r_s \lesssim 6$), attention must be paid also to the behaviour of the pair function $g(r)$ at short distance. It has been shown by Kimball¹⁶⁾ that the derivative of $g(r)$ at the origin $r = 0$ obeys the relation

$$\left. \frac{dg(r)}{dr} \right|_{r=0} = g(0)/a_0, \quad (2.4)$$

the value of $g(0)$ being finite as a consequence of quantal tunnelling. From the work of Niklasson¹⁷⁾ the relation (2.4) determines also the approach of the structure factor $S(k)$ to its asymptotic value of unity at large k , since

$$\lim_{k \rightarrow \infty} \{ k^4 [S(k) - 1] \} = -8\pi n \left. \frac{dg(r)}{dr} \right|_{r=0}. \quad (2.5)$$

Accurate results for $g(0)$ as a function of r_s have been reported by Yasuhara¹⁸⁾ from an evaluation of ladder diagrams, leading to the formula

$$g(0) = \frac{1}{8} \left[x / I_1(x) \right]^2 \quad (2.6)$$

where $x = 1.629 r_s^{1/2}$ and $I_1(x)$ is the modified Bessel function of the first order.

The structural properties that we have recalled above for the degenerate electron fluid can be preserved by choosing an effective pair potential of the form

$$\bar{\Phi}(r) = \frac{e^2}{r} \left[1 - \exp(-zr) \cos(\alpha r) \right] \quad (2.7)$$

for its classical equivalent at an effective temperature given by Eq. (2.3). Here, z and α are parameters to be determined from the Kimball-Niklasson relation (2.4) and from Yasuhara's values for $g(0)$ in the degenerate fluid.

2.1 Structure of jellium at metallic densities

The form (2.7) of the effective electron-electron potential has the further advantage that it allows an analytic evaluation of the structure of the electron fluid in the range of relatively low coupling which is of present interest. This is obtained by using the Debye-Hückel integral equation for liquid structure¹⁹⁾,

$$h(r) = -\bar{\Phi}(r)/E + n \int d\varepsilon' h(\varepsilon - \varepsilon') \bar{\Phi}(r')/E, \quad (2.8)$$

where $h(r) = g(r) - 1$ and

$$E = \frac{1}{2} \hbar \omega_p = \left(3/r_s^3\right)^{1/2} R_{yd}. \quad (2.9)$$

Equation (2.8) is easily solved in Fourier transform for the structure factor $S(k)$, given by

$$S(k) = 1 + (4\pi n/k) \int_0^\infty dr \sin(kr) r h(r). \quad (2.10)$$

The result is

$$S(k) = \frac{k^6 + 2(z^2 - \alpha^2)k^4 + (z^2 + \alpha^2)^2 k^2}{k^6 + 2(z^2 - \alpha^2)k^4 + [(z^2 + \alpha^2)^2 + k_s^2(z^2 - \alpha^2)]k^2 + k_s^2(z^2 + \alpha^2)^2}, \quad (2.11)$$

with

$$k_s^2 = 4\pi n e^2 / E = 2(3/r_s^3)^{1/2} / \alpha_0^2. \quad (2.12)$$

This expression satisfies Eq. (2.1) and yields

$$\lim_{k \rightarrow \infty} \{k^4 [S(k) - 1]\} = -k_s^2 (z^2 - \alpha^2). \quad (2.13)$$

The pair function $g(r)$ is evaluated by Fourier inversion of Eq. (2.11)

as

$$g(r) = 1 + (k_s^2 / 4\pi n r) \sum_{\ell=1}^3 A_\ell \exp(-a_\ell r) \quad (2.14)$$

where a_ℓ^2 are the roots of the cubic equation in the variable k^2 which is obtained by setting the denominator in Eq. (2.11) equal to zero. One of these roots is real and the others are complex conjugate. The quantities A_ℓ are given by

$$A_1 = \left[\alpha_1^2 (z^2 - \alpha^2) - (z^2 + \alpha^2)^2 \right] / \left[(\alpha_1^2 - \alpha_2^2)(\alpha_1^2 - \alpha_3^2) \right] \quad (2.15)$$

etcetera. For $r \rightarrow 0$ one easily finds

$$g(0) = 1 - (k_s^2 / 4\pi n) \sum_{\ell=1}^3 A_\ell a_\ell \quad (2.16)$$

and

$$\left. \frac{dg(r)}{dr} \right|_{r=0} = (k_s^2 / 4\pi n) \sum_{\ell=1}^3 A_\ell a_\ell^2 = k_s^2 (z^2 - \alpha^2) / 8\pi n. \quad (2.17)$$

We see by comparison of Eq. (2.17) with Eq. (2.13) that Eq. (2.5) is satisfied. Eqs. (2.16) and (2.17) determine the parameters z and α in the effective potential through the use of Eqs. (2.4) and (2.6).

Fig. 1 reports our results for the structure factor $S(k)$ of the degenerate electron fluid at two values of r_s spanning the range of metallic densities, while Fig. 2 shows the corresponding pair function $g(r)$. Comparison is shown in these figures with the results obtained by Lantto¹³⁾ in the quantal (Fermi) hypernetted chain approximation (FHNC). It should be noticed that Lantto's results are in good agreement with those obtained by alternative and wholly independent quantal evaluations, namely from the theory of the dielectric response function of the degenerate electron fluid¹²⁾ and from quantal simulation techniques¹⁴⁾.

We can therefore conclude from the comparisons shown in Figs. 1 and 2 that our simple approach yields good approximate results for the structure of the degenerate electron fluid in the metallic density range. Of course, the Debye-Hückel approximation becomes invalid with increasing coupling strength and a better theory of classical liquid structure should be used at values of r_s larger than considered here.

3. EFFECTIVE PAIR POTENTIALS IN LIQUID METAL AND PERTURBATIVE THEORY OF STRUCTURE

At variance from Eq. (2.1), the partial structure factors $S_{\alpha\beta}(k)$ for electrons and ions in a pure liquid metal are related in the long wavelength limit to the isothermal compressibility K_T by electroneutrality, according to 2),3)

$$\lim_{k \rightarrow 0} \left[Z^{-1} S_{ee}(k) = Z^{-1/2} S_{ei}(k) = S_{ii}(k) \right] = n_i k_B T K_T \quad (3.1)$$

where Z is the ionic valence and $n_i = n/Z$ is the ionic density. As discussed by Tosi and March⁴⁾, if one defines partial direct correlation functions $c_{\alpha\beta}(k)$ through the relations

$$c_{\alpha\beta}(k) = \delta_{\alpha\beta} - \sum_{\alpha\beta}^{-1}(k) \quad (3.2)$$

involving the inverse of the matrix of partial structure factors, then Eqs. (3.1) require that $c_{\alpha\beta}(k)$ have in the extreme long wavelength limit the asymptotic forms

$$c_{ii}(k) \rightarrow -4\pi n_i Z^2 e^2 / k^2 E, \quad (3.3)$$

$$c_{ie}(k) \rightarrow 4\pi (n_i n_e)^{1/2} Z e^2 / k^2 E \quad (3.4)$$

and

$$c_{ee}(k) \rightarrow -4\pi n_e e^2 / k^2 E. \quad (3.5)$$

In these equations E is a common characteristic energy, which in the light of the results given in Sec. 2 is naturally chosen as determined by Eq. (2.9). From Eqs. (3.2)-(3.5) we then find

$$\lim_{k \rightarrow 0} [Z S_{ii}(k) + S_{ee}(k) - 2 Z^{1/2} S_{ie}(k)] = k^2 / k_s^2, \quad (3.6)$$

an approximate relation derived by Tosi and March⁴⁾ on the assumption that the long wavelength behaviour of the partial structure factors in the liquid metal is determined by collective modes. These are sound waves [Eq. (3.1)] and plasma waves [Eq. (3.6)].

In a classical Coulomb liquid at temperature T , on the other hand, the Ornstein-Zernike direct correlation functions are asymptotically related to the Coulombic tails of the pair potentials $\varphi_{\alpha\beta}(k)$ by

$$\lim_{k \rightarrow 0} [c_{\alpha\beta}(k) = -(n_\alpha n_\beta)^{1/2} \varphi_{\alpha\beta}(k) / k_B T]. \quad (3.7)$$

Comparison of Eq. (3.7) with Eq. (3.3)-(3.5) shows that the effective pair potentials $\Phi_{\alpha\beta}(k)$ in a pseudoclassical description of the liquid metal at temperature T should have Coulombic tails which are scaled by the factor $k_B T / E$ relative to those of the true pair potentials.

The above prescription for the Coulombic tails in $\Phi_{\alpha\beta}(k)$ should be supplemented by a model for the ionic cores. The simplest model that one may consider assumes hard spheres for the ion core-ion core interactions and the empty core model of Ashcroft²⁰⁾ for the electron-ion core interactions. Thus, our model for the liquid metal at temperature T is summarized by the following expressions for the effective pair potentials:

$$\Phi_{ii}(r) = \begin{cases} \infty & (r < \sigma) \\ Z^2 e^2 k_B T / r E & (r > \sigma) \end{cases} \quad (3.8)$$

$$\Phi_{ie}(r) = \begin{cases} 0 & (r < r_c) \\ -Z e^2 k_B T / r E & (r > r_c) \end{cases} \quad (3.9)$$

and

$$\Phi_{ee}(r) = (e^2 k_B T / r E) [1 - \exp(-zr) \cos(\alpha r)]. \quad (3.10)$$

Here, σ and r_c are parameters of the ionic cores while z and α are parameters already determined in Sec. 2.

3.1 Perturbative treatment of the electron-ion coupling

In view of the smallness of the electron-ion coupling in Eq. (3.9), a useful approximate solution for the structure of the model can be obtained even for polyvalent metals by a perturbative switching of this coupling onto two independent "reference liquids" described by the effective pair potentials (3.8) and (3.10). The electronic reference liquid has structure factor $S(k)$ as evaluated in Sec. 2. The ionic reference liquid is a classical plasma of charged hard spheres with structure factor $S_{ii}^{(0)}(k)$ say.

In a first-order generalized cluster expansion^{21),19)} (or random phase approximation, RPA) the partial structure factors of the model are given by

$$S_{ee}(k) = S(k)/D(k), \quad (3.11)$$

$$S_{ii}(k) = S_{ii}^{(0)}(k)/D(k) \quad (3.12)$$

and

$$S_{ie}(k) = -(n_i n_e)^{1/2} \frac{\Phi_{ie}(k)}{k_e \tau} S(k) S_{ii}(k) / k_e \tau \quad (3.13)$$

where

$$D(k) = 1 - n_i n_e \left[\frac{\Phi_{ie}(k)}{k_e \tau} \right]^2 S(k) S_{ii}^{(0)}(k). \quad (3.14)$$

Of course, an optimized perturbative treatment of the coupling (3.9), along the lines of the work of Weeks *et al.*²²⁾, would be necessary for an evaluation of the pair distribution functions $g_{\alpha\beta}(r)$ at short distances.

On the other hand, the RPA solution in Eqs. (3.11)-(3.14) yields analytic expressions for the partial structure factors of the model when it is combined with known analytic results for the liquid of charged hard spheres in the mean spherical approximation^{23),24)}. The corresponding analytic form of $S_{ii}^{(0)}(k)$ is reported for completeness in the Appendix. We give here for later use only the expression for the isothermal compressibility of the liquid metal that we obtain from Eq. (3.1) using Eqs. (3.11)-(3.14) and the analytic form of $S_{ii}^{(0)}(k)$ in the Appendix. This is

$$n k_e \tau \kappa_T = \left(k_2^2/k_e^2 + k_3^2/k_i^2 + k_3^2 r_c^2 \right)^{-1} \quad (3.15)$$

where

$$k_e^2 = k_3^2 (z^2 + \alpha^2) / [(z^2 + \alpha^2)^2 - k_3^2 (z^2 - \alpha^2)] \quad (3.16)$$

and

$$k_i^2 = \sum k_j^2 / Q_0^2, \quad (3.17)$$

the quantity Q_0^2 being defined in the Appendix in terms of structural parameters of the liquid of charged hard spheres.

4. RESULTS FOR SODIUM AND BERYLLIUM

Our main interest in this section will be to evaluate how the electron-electron structure factor in jellium, that we have calculated in Sec. 2, is modified when a weak electron-ion interaction is switched on perturbatively.

Let us consider first the case of liquid sodium near freezing at atmospheric pressure, i.e. at temperature $T = 371$ K and density $n_1 = n = 0.0242 \text{ \AA}^{-3}$, corresponding to $r_s = 4.05$. The parameters of the model are the empty core radius r_c and the ionic diameter σ . For the former we adopt the value $r_c = 0.89 \text{ \AA}$ as deduced from a fit of phonon dispersion curves in crystalline sodium²⁵⁾. For what concerns the bare ion core-ion core interactions, on the other hand, our model is closely related to neutral-hard-sphere models of the structure of liquid metals. We therefore adopt the value $\sigma = 3.3 \text{ \AA}$ from the work of Ashcroft and Lekner²⁶⁾, which corresponds to a packing fraction $\eta = \frac{1}{6} \pi n_1 \sigma^3$ of about 0.45. Ashcroft and Lekner show that the structure factor of a liquid of neutral hard spheres with this choice of diameter, when calculated in the Percus-Yevick approximation, agrees reasonably well with the measured structure factor. Bearing also in mind that the mean spherical approximation for a liquid of charged hard spheres goes into the Percus-Yevick approximation when the charges are switched off, we expect that $S_{ii}^{(0)}(k)$ with the above choice for σ will already show the main features of the observed ion-ion structure factor, except near the origin where $S_{ii}^{(0)}$ vanishes proportionally to k^2 .

The above expectation is confirmed by the results shown in Fig. 3, which reports $S_{ii}^{(0)}(k)$ and $S_{ii}(k)$ for sodium in comparison with the structure factor determined by Greenfield *et al.*²⁷⁾ from X-ray diffraction experiments. All the structure factors in this figure have been magnified by a factor ten in the small-angle scattering region. We see that the main effect of electronic screening is taking place at small k , where it corrects the parabolic behaviour of $S_{ii}^{(0)}(k)$ to give the "screened" structure factor $S_{ii}(k)$ in good agreement with experiment. In particular, we find $S_{ii}(k \rightarrow 0) = 0.0237$ from Eq. (3.15), which is in excellent agreement with the measured value of the isothermal compressibility. We shall return on this point in the next section, when we shall attempt a critique of our pseudo-classical approach. For the present we note that the value of the right-hand side of Eq. (3.15) is largely determined in our calculation by the hard-core term given by Eq. (3.17).

With regard to the comparison of $S_{ii}(k)$ at intermediate and large k with experiment in Fig. 3, we notice some discrepancies arising both from our use of the mean spherical approximation and from our non-optimized choice of the value of σ in the presence of Coulombic repulsive tails in the bare ion-ion potential. Of course, we are in the present context mainly interested in using $S_{ii}^{(0)}(k)$ and $S_{ii}(k)$ as approximate input for the evaluation of the electron-electron and electron-ion structure factors. Better calculations than the present one exist already in the literature for the ion-ion correlations in the liquid alkalis from an electron-ion plasma viewpoint⁸⁾.

Fig. 4 and 5 report $S_{ie}(k)$ and $S_{ee}(k)$ for liquid sodium as calculated in our approach. The two main structures in $S_{ie}(k)$ in Fig. 4 correspond to the two main peaks in $S_{ii}(k)$. They therefore describe some relative order of the electronic fluid induced by the ionic fluid. The net effect on the X-ray scattered intensity in a diffraction experiment is nevertheless quite small, being of the order of 2% at the main peak of $S_{ii}(k)$. Earlier calculations of $S_{ie}(k)$ by Chihara³⁾, using a set of integral equations derived from a generalized Hartree approximation, showed a behaviour similar to our own for $k \leq k_F$, but indicated that this function is very small above the Fermi wavenumber k_F .

Our results for $S_{ee}(k)$ in sodium in Fig. 5 agree qualitatively with earlier theoretical results, and in particular with those of Cusack *et al.*⁵⁾, to the effect that relatively minor changes are induced by the presence of the ions in this function relative to the structure factor of the jellium model. The main effects are the emergence of a finite value for $S_{ee}(k \rightarrow 0)$, in accord with Eq. (3.1), and the appearance of a broad maximum in the region of the main peak in $S_{ii}(k)$. The corresponding contribution to the X-ray scattered intensity in a diffraction experiment is again quite small.

For a test of the reasonableness of our results for $S_{ee}(k)$ we must turn to the case of liquid beryllium near freezing. We take $T = 1550$ K and $n_i = \frac{1}{2} n = 0.124 \text{ \AA}^{-3}$, i.e. $r_s = 1.87$, and choose $\sigma = 1.90 \text{ \AA}$, corresponding to $\eta = 0.45$. We estimate $r_c = 0.52 \text{ \AA}$ both by a linear extrapolation of the results of Price *et al.*²⁵⁾ for r_c versus r_s in the alkalis and by assuming proportionality to atomic orbital radii²⁸⁾. Fig. 6 reports $S(k)$ and $S_{ee}(k)$ for this system, in comparison with the electron-electron structure factor determined experimentally for crystalline beryllium by Eisenberger *et al.*⁹⁾ from X-ray inelastic scattering experiments, using

suitable filters of the scattered radiation to separate out the quasielastic component. It is evident from the figure that, although the difference between $S_{ee}(k)$ and $S(k)$ is again quite small, the "screened" electron-electron structure factor follows the trend of the data much better than the jellium structure factor, the overall agreement between theory and experiment being in fact rather good.

5. SUMMARY AND DISCUSSION

Some confidence in our approach has been gained from three main sets of results: (i) the electronic structure factor $S(k)$ of jellium in the metallic density range and the corresponding electron pair distribution function $g(r)$ are in good agreement with the results of fully quantal evaluations, the latter being quite reliable because of consistency between the predictions made by several independent techniques; (ii) the partial ion-ion structure factor $S_{ii}(k)$ compares with experiment at a similar level of quality as the results of hard sphere models; and (iii) the partial electron-electron structure factor $S_{ee}(k)$ reproduces at least semi-quantitatively the broad peak observed by Eisenberger *et al.*⁹⁾ for crystalline beryllium.

In concluding this paper, we wish to comment specifically on some limitations of a simple pseudoclassical treatment of the degenerate electron fluid. It is evident that the interacting degenerate fluid possesses two characteristic energy scales, i.e. the zero point energy $\frac{1}{2} \hbar \omega_p$ of the plasmon excitation and the Fermi energy E_F . Although only the first of these has been explicitly built into our pseudoclassical model, it is fortunate that these characteristic energies are comparable over the metallic density range. Clearly, however, our approach should not be extended to much lower values of r_s , where the effects from Fermi statistics are becoming dominant and are being included only through our fit of the value of $g(0)$.

Even in the metallic density range, an explicit evaluation of the compressibility of jellium from the k^4 term in the low- k expansion of $S(k)$ in Eq. (2.11) shows large errors in this quantity as compared with the results of reliable quantal evaluations. These errors would become apparent in our calculation of the compressibility of the liquid metal, were it not for the fact that our formula (3.15) is dominated by the ion-ion term. Nevertheless, as our evaluation of the partial structure factors by linear

response theory illustrates, $S(k)$ in a pseudoclassical model should have the dual role of a structural function and of a dielectric screening function. Therefore, at the present level of approximation the screening of the ions by the electrons, and more specifically the electron-ion structure factor $S_{ie}(k)$ in Fig. 4, should be regarded with great caution.

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APPENDIX

Structure factor of the liquid of charged hard spheres in the mean spherical approximations

The structure factor $S_{ii}^{(0)}(k)$ of the liquid of charged hard spheres is easily evaluated analytically in the mean spherical approximation from the results reported by Parrinello and Tosi²⁴⁾. We find

$$S_{ii}^{(0)}(k) = [Q(k)Q(-k)]^{-1} \quad (A.1)$$

where the Baxter matrix $Q(k)$ is given explicitly by

$$Q(k) = 1 - n_i \left[(ZA/ik) + Q' \varphi_1(k) + Q'' \varphi_2(k) + \pi Z n_i A \varphi_3(k) \right], \quad (A.2)$$

with

$$\begin{cases} \varphi_1(k) = (ik)^{-2} [1 + ik\sigma - \exp(ik\sigma)] \\ \varphi_2(k) = -(ik)^{-3} [1 + ik\sigma + \frac{1}{2}(ik\sigma)^2 - \exp(ik\sigma)] \\ \varphi_3(k) = 2(ik)^{-4} [1 + ik\sigma + \frac{1}{2}(ik\sigma)^2 + \frac{1}{6}(ik\sigma)^3 - \exp(ik\sigma)]. \end{cases} \quad (A.3)$$

The parameters in Eq. (A.2) are given by

$$Q' = 2\pi\sigma \left(1 + \frac{1}{2}\gamma\right) (1-\gamma)^{-2} - 2\gamma^2 A^2 / \lambda^2, \quad (A.4)$$

$$Q'' = 2\pi(1+2\gamma)(1-\gamma)^{-2} + 2\pi\gamma\sigma n_i A / \lambda^2 (1-\gamma) \quad (A.5)$$

and

$$A = \left(Z \lambda^2 / 2\gamma \right) (1-\gamma) \left[\gamma\sigma + (1+2\gamma)/(1-\gamma) \right]^{-1}, \quad (A.6)$$

where $\eta = 1 - \pi n_i \sigma^3 / 6$ is the packing fraction, $\lambda^2 = 4\pi e^2 / E$ is a measure of the strength of the interaction in units of the characteristic energy E introduced in Eq. (2.9), and γ is given by²³⁾

$$\gamma \sigma = -\frac{1}{2} \frac{1+\eta}{1-\eta} \left\{ 1 - \left[1 + 2\kappa \frac{(1-\eta)^3}{(1+\eta)^3} \right]^{1/2} \right\} \quad (\text{A.7})$$

with $\kappa^2 = n_1 Z^2 \lambda^2 \sigma^2$.

The parameter Q_0^2 entering Eq. (3.17) is determined from the long-wavelength limit of Eq. (A.1) and is given by

$$Q_0^2 = \left[1 + n_i \left(\frac{1}{2} \sigma^2 Q^i - \frac{1}{6} \sigma^3 Q'' + \frac{1}{12} \sigma^4 \pi Z n_i A \right) \right]^2 + 2 Z n_i^2 A \left[\frac{1}{2} \sigma^2 Q^i - \frac{1}{24} \sigma^4 Q'' + \frac{1}{60} \sigma^5 \pi Z n_i A \right]. \quad (\text{A.8})$$

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FIGURE CAPTION

- Fig. 1 Electronic structure factor $S(k)$ in jellium at $r_s = 1$ (left) and $r_s = 5$ (right) versus kr_0 , with $r_0 = r_s a_0$. Solid curves: present results; dashed curves: from FHNC results of Lantto ¹³.
- Fig. 2 Electron pair distribution function $g(r)$ in jellium at $r_s = 1$ (left) and $r_s = 5$ (right) versus r/r_0 . Solid curves: present results; dashed curves: from FHNC results of Lantto ¹³.
- Fig. 3 Ion-ion structure factor in liquid sodium near freezing versus kr_0 , before and after screening by the conduction electrons (dashed and solid curve, respectively). Dots are from X-ray diffraction experiments of Greenfield et al. ²⁷.
- Fig. 4 Electron-ion structure factor $S_{ie}(k)$ in liquid sodium near freezing.
- Fig. 5 Electron-electron structure factor $S_{ee}(k)$ in liquid sodium near freezing (solid curve), compared with the electronic structure factor in jellium at the same density (dashes).
- Fig. 6 Electron-electron structure factor $S_{ee}(k)$ in liquid beryllium near freezing (solid curve) and electronic structure factor in jellium at the same density (dashes), compared with the observed electronic structure factor in crystalline beryllium from inelastic X-ray scattering experiments of Eisenberger et al. ⁹) (dots, as read from Fig. 2 in Ref. 9).

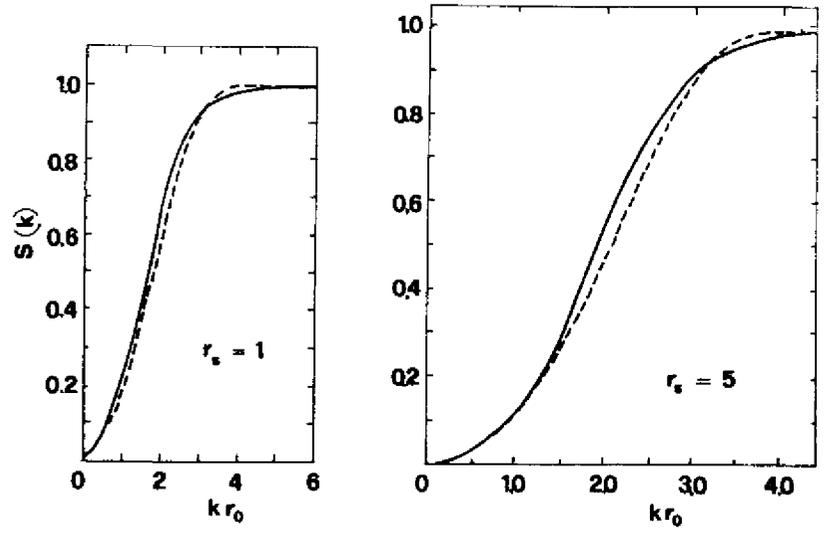


Fig. 1

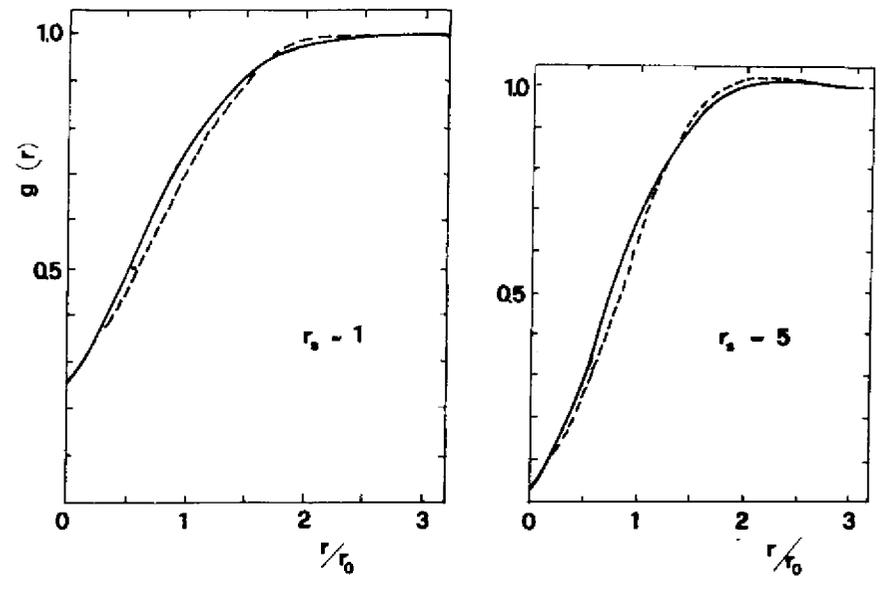


Fig. 2

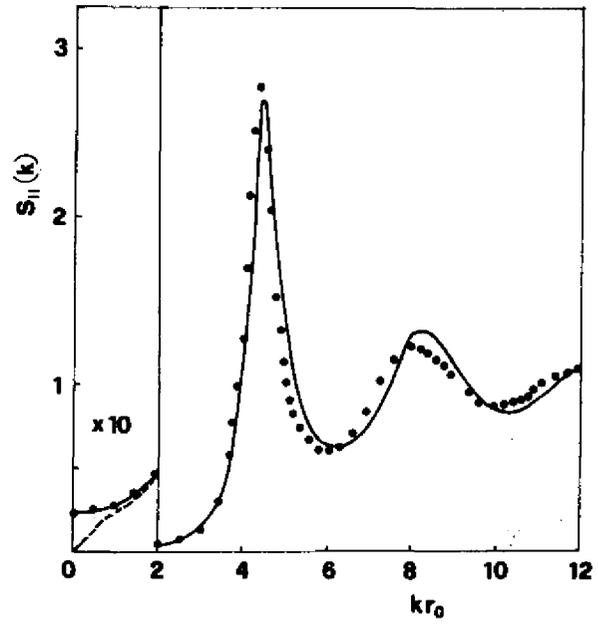


Fig. 3

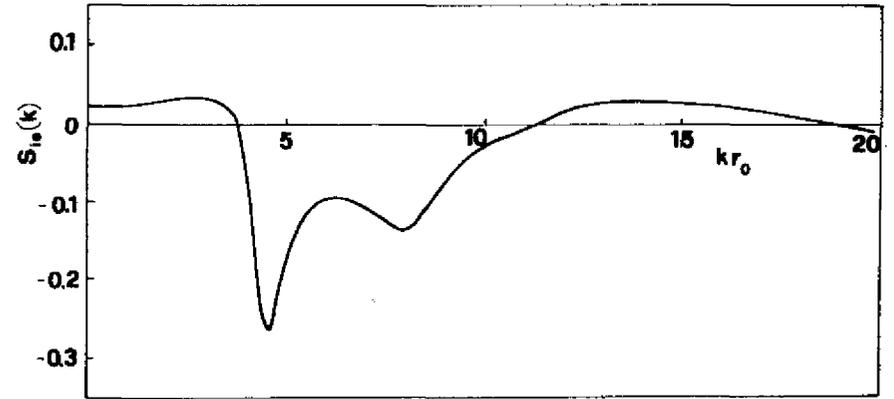


Fig. 4

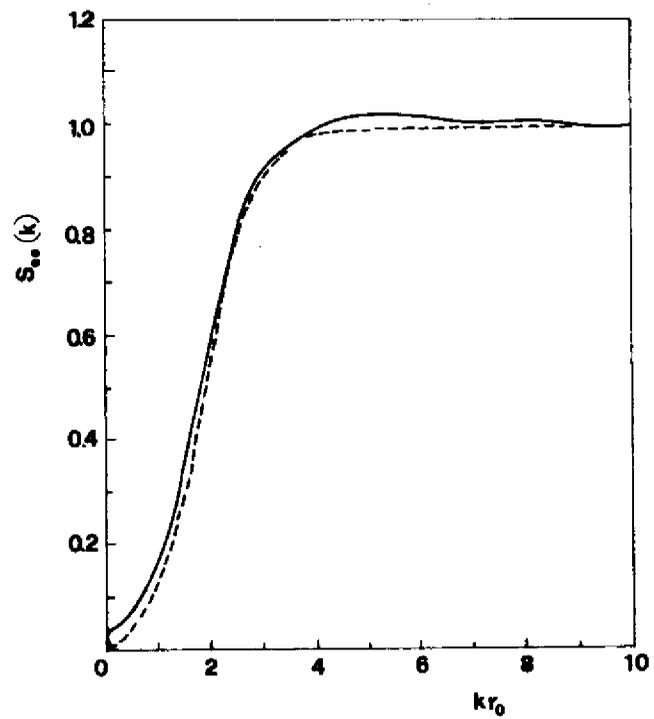


Fig. 5

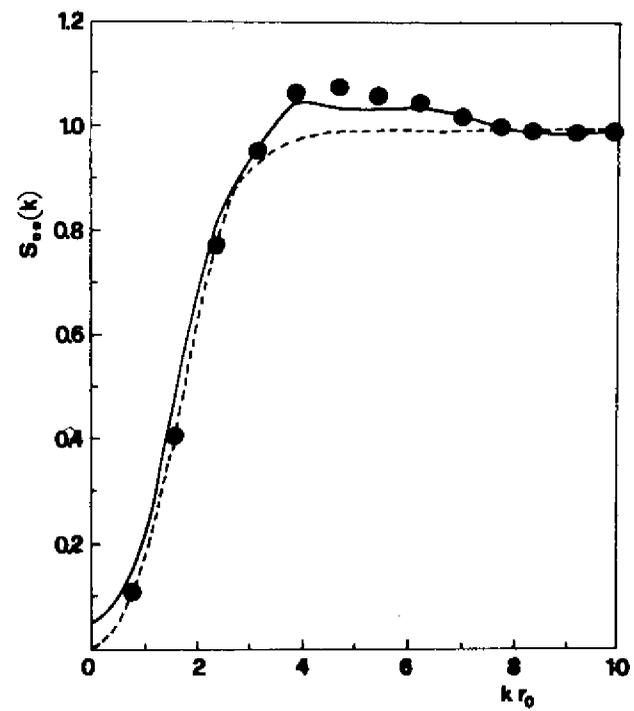


Fig. 6