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# OPTIMIZED RANDOM PHASE APPROXIMATION FOR THE STRUCTURE OF LIQUID ALKALI METALS AS ELECTRON-ION PLASMAS*

G. Senatore and M.P. Tosi
International Centre for Theoretical Physics, Trieste, Italy
and
GNSM-CNR, Istituto di Fisica Teorica dell'Università, Trieste, Italy

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In a previous publication[1] we have shown that the model of the one-component classical plasma on an inert background (OCP) provides a basis for calculating the liquid structure factor of the alkali metals. This was achieved by allowing the conduction electrons to screen the structure of the OCP through the formalism of linear screening theory, but an empirical cut-off of the screening correction at the first node of the electron-ion pseudopotential in wavenumber space was found to be necessary. The purpose of this letter is to stress that the above results point the way towards an unconventional optimized-random-phase-approximation (ORPA) approach[2] to the structure of these liquid metals, and in fact provide already a good first-order solution for such an approach.

Linear screening theory in its simplest formulation leads,



as is well known, to the following expression for the Fourier transform of the effective ion-ion potential in the alkali metal,

$$V(k) = \frac{4\pi e^2}{k^2} + \tilde{v}(k). \qquad (1)$$

The first term in this expression, i.e. the ion-ion Coulomb repulsion, determines the structure of the OCP, while the screening correction $\tilde{v}(k)$ is given by

$$\tilde{v}(k) = \frac{V_{ei}^2(k)}{4\pi e^2/k^2}\left[\frac{1}{\varepsilon(k)} - 1\right], \qquad (2)$$

in terms of the bare electron-ion pseudopotential $V_{ei}(k)$ and of the dielectric function $\varepsilon(k)$ of the electron gas. The term $\tilde{v}(k)$, as e.g. evaluated for the alkali metals by Price et al[3], provides a purely attractive interaction between the ions. The only source of repulsive interionic forces in such an approach is thus the bare Coulomb term.

The crucial point for the following discussion is that, at the bare ion-ion coupling strengths that are appropriate for liquid alkali metals, the structure of the OCP determined by the Coulomb repulsion is described with very high accuracy[4] by a charged-hard-spheres (CHS) model, provided that this model is required to reproduce the thermodynamic properties of the OCP. In particular, one can introduce an effective CHS diameter $\sigma$ within which the radial distribution function of the bare OCP practically vanishes, the value of $\sigma$ being determined[5] through the virial theorem for the OCP. Keeping this result in

mind, let us examine the expression yielded by linear screening theory for the structure factor S(k) of the liquid metal,

$$S(k) = S_0(k) \Big/ \left[1 + \frac{\rho \tilde{v}(k)}{k_B T} S_0(k)\right] , \qquad (3)$$

where $S_0(k)$ is the structure factor of the OCP. In the usual language of liquid structure theory[2], this expression can then be viewed as combining the CHS-like structure of the strongly coupled OCP with a random-phase-approximation (RPA) on the attractive screening correction $\tilde{v}(k)$. Such a treatment is appropriate and quite accurate[1] in the small angle scattering region, but is breaking down as one approaches the main peak of S(k).

An optimization of the RPA leading to eqn (3), analogous in spirit to the ORPA that has been developed[2] for atomic liquids, suggests itself at this point. Since the ions of the liquid metal should not penetrate into the CHS effective hard core, the potential $\tilde{v}(k)$ in eqn (3) can be replaced by the Fourier transform of an effective potential $\tilde{v}_{eff}(r)$ having the ORPA properties, i.e. such that (a) it differs from $\tilde{v}(r)$ only inside the hard core region, and (b) it leads to a vanishing radial distribution function g(r) for the liquid metal inside the same region. This procedure introduces the effect of the attractive interaction in the region of space where it is felt, without modifying the excluded volume effect due to the Coulomb repulsive interaction.

To show that the empirical cut-off in $\tilde{v}(k)$ adopted in ref. 1 is a close realization of an ORPA approach as outlined above,



it thus remains for us to show that the truncated form of $\tilde{v}(k)$ ($\tilde{v}_t(k)$, say) closely satisfies the properties (a) and (b). An illustration is presented in figures 1 and 2 for the case of potassium near freezing. Experimental results[6] for g(r) are also reported in figure 2 for comparison. The discrepancies between $\tilde{v}_t(r)$ and the effective potential $\tilde{v}_{eff}(r)$ of the suggested ORPA scheme for liquid alkali metals should clearly be minor ones, at least from a practical point of view.

It should also be noted from figure 1 that in the region $r \lesssim \sigma$, where the total potential V(r) (given by the difference between the full curve and the dash-dot curve) has become repulsive, the Coulomb repulsive term is varying in a considerably more rapid manner than the screening attractive term. This justifies an approach which combines an accurate treatment of the former with an ORPA treatment of the latter. The cancellation between the two terms at large values of r is ensured by eqn (3). The exact fulfilment of the properties (a) and (b) may be expected to lead to a somewhat less abrupt truncation of the screening term $\tilde{v}(k)$ than adopted in ref. 1, and possibly to some reduction of S(k) below $S_0(k)$ in the region of its main peak.

We should explicitly point out, in conclusion, that the 'hard core' in the CHS model entering our scheme has the property[5] that the radial distribution function vanishes continuously for $r = \sigma$. A conventional ORPA approach to the liquid metal as

constituted of pseudoatoms must instead tackle also the softening of the neutral-hard-spheres repulsion, which introduces a discontinuous drop in the initial g(r) at contact.

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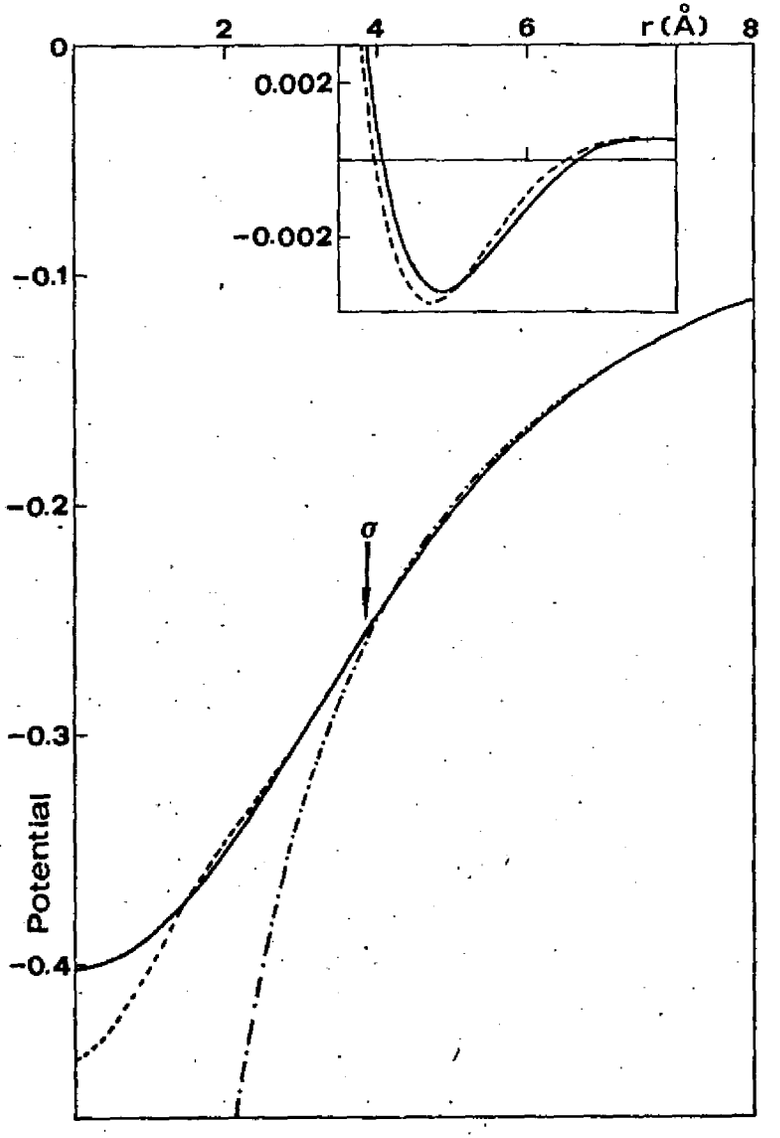
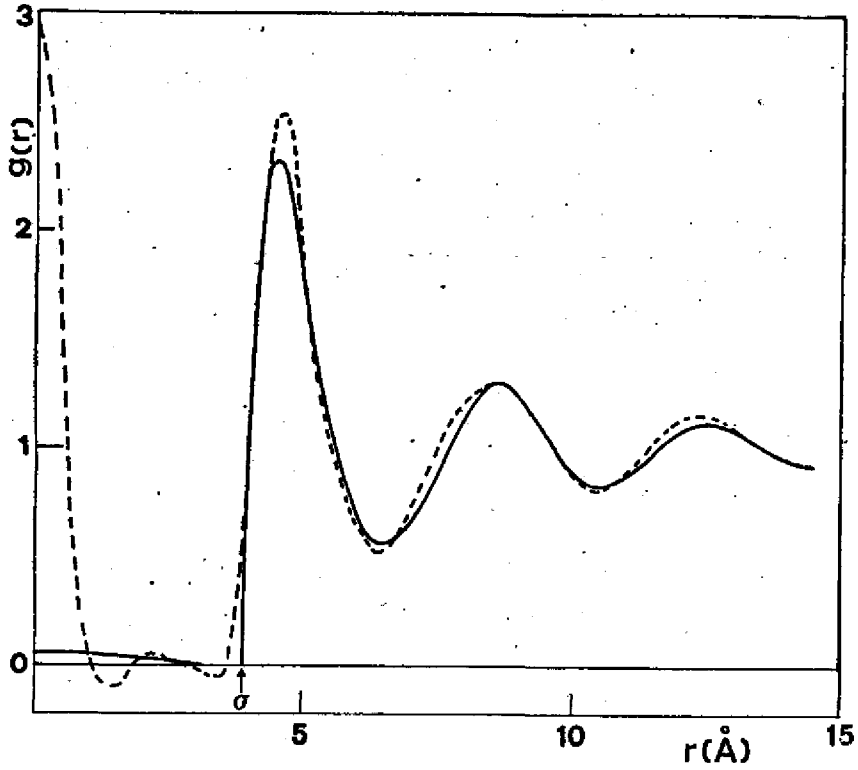
Figure captions

Figure 1. Illustrating the ORPA property (a) for the truncated potential $\tilde{v}_t(r)$ of ref. 1 (full curve) when compared with the potential $\tilde{v}(r)$ of eqn (2) (dashed curve). The arrow marks the CHS diameter $\sigma$ for the OCP. The dot-dash curve reports for comparison the Coulomb potential $-e^2/r$. The inset shows on an enlarged vertical scale the total ion-ion potential in the region of its main minimum, as calculated from $\tilde{v}_t(r)$ (full curve) and from $\tilde{v}(r)$ (dashed curve). All potentials are in units of $e^2/\text{Å}$ and refer to liquid potassium at 65°C.

Figure 2. Illustrating the ORPA property (b) for the truncated potential $\tilde{v}_t(r)$ of ref. 1. The full curve is the corresponding radial distribution function $g(r)$ for liquid potassium at 65°C. The experimental data (dashed curve) are from M.J. Huijben and W. van der Lugt (ref. 6): the deviations from zero at small r result from the truncation of the experimental structure factor at large k.







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