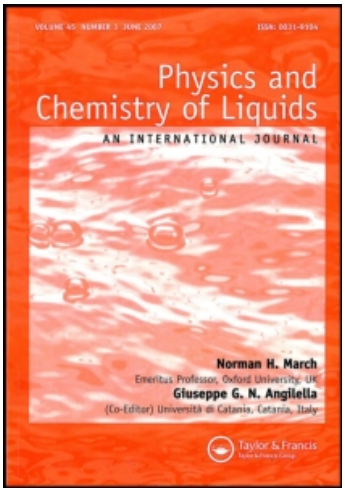

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Letter

STRUCTURE AND PHYSICAL PROPERTIES OF Li-H PLASMA

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An approach to static and dynamic structure of Li-H plasma in different ionization states is set out, long wave properties being emphasized.

Keywords: Binary liquid metal mixtures; electron-ion structure factor

There continues in the area of plasmas to be some interest in Li-H, and in particular its physical properties in different ionization states.

In this Letter we shall discuss, therefore, without presenting detailed calculations, some aspects of Li-H plasmas. Let us begin with the fully ionized Li^{3+}-H^{+} plus neutralizing electrons. In this context, it is relevant that Stevenson [1] proposed that He^{2+}-H^{+} mixtures in a responsive electronic background phase separate under conditions of temperature and pressure characteristic of the interior of Jupiter.

In Stevenson's work the ions were described by a hard-sphere reference system plus thermodynamic perturbation theory. The response of the electron liquid was 'mimicked' using dielectric screening according to Hubbard [2] and Geldart and Vosko [3]. Following Stevenson's study, Hansen *et al.* [4] presented numerical results for thermodynamic properties and equilibrium structure, with neutralization by a rigid uniform background of electrons. While the

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structural data presented were for the ionic charge ratio $z_B/z_A = 2$ considered by Stevenson, thermodynamic data were discussed for $z_B/z_A = 3$. Quantum corrections, plus effects of the polarization of the electronic background by the ions were then dealt with perturbatively.

It is immediately relevant to Li^{3+}-H^{+} mixtures that in their Figure 4 Hansen *et al.* [4] show phase separation curves, by plotting T against mixture concentration, for comparison with He^{2+}-H^{+} mixtures. They emphasize that the most striking difference between the two sets of coexistence curves is the order of magnitude increase of the critical temperature of demixing in changing from He^{2+} to Li^{3+}.

As to structure, for equal concentrations of ions A and B with $z_A = 1$ and $z_B = 2$ in a non-responsive electronic background, at plasma parameter Γ, defined by

$$\Gamma = \frac{e^2}{ak_B T} \tag{1}$$

with a the ion sphere radius, set equal to 40, the three pair distribution functions $g_{\alpha\beta}(r)$ are plotted from hypernetted chain calculations and compared with the results of Monte Carlo computer experiments (see Fig. 2 of Hansen *et al.* [4]). The higher charge species, $g_{BB}(r)$ shows more pronounced structure than $g_{AB}(r)$ and $g_{AA}(r)$ and this feature can be expected to be enhanced for charge ratio z_B/z_A appropriate to Li^{3+}-H^{+}.

March *et al.* [5] generalized to binary liquid metal mixtures the screening conditions

$$S_{ic}(q = 0) = z^{1/2} S(q = 0) \tag{2}$$

and

$$S_{ee}(q = 0) = z S(q = 0) \tag{3}$$

derived by Chihara [6] and independently by Watabe and Hasegawa [7] and relating the ion-electron and electron-electron structure factors in a liquid metal to the ion-ion structure factor. Their argument was, essentially, to sit successively on ion A, ion B and an electron. In each case, they calculated from the radial distribution functions the total charge around the chosen species at the origin and

required that species to be perfectly screened. As an example of their results we record the electron–electron structure factor $S_{ee}(q)$ at $q=0$ (simply denoted S_{ee} etc. below), namely

$$S_{ee} = z_A^2 \frac{n_A}{n_e} S_{AA} + 2z_A z_B \frac{(n_A n_B)^{1/2}}{n_e} S_{AB} + z_B^2 \frac{n_B}{n_e} S_{BB} \tag{4}$$

where z_A and z_B are the valences of ions A and B respectively, while n_A and n_B are the ionic number densities.

We now apply eqn (4), and its analogues for S_{Ae} and S_{Be} again at $q=0$, to the specific case of Li^{3+}-H^+ with equal concentration of ions. The results are

$$S_{ee} = \frac{9}{4} S_{LiLi} + \frac{3}{2} S_{LiH} + \frac{1}{4} S_{HH}, \tag{5}$$

$$S_{Le} = \frac{3}{2} S_{LiLi} + \frac{1}{2} S_{LiH} \tag{6}$$

and

$$S_{He} = \frac{3}{2} S_{LiH} + \frac{1}{2} S_{HH}. \tag{7}$$

To our knowledge, no data for valences 3 and 1 are presently available for binary liquid metal mixtures. However, the partially ionized plasma Li^+-H^+ is also of interest in the present contest. Here, it is relevant to mention that March *et al.* [5] have used thermodynamic data for the long wavelength limit of the ionic structure factors to construct the electronic structure factors in the liquid Na-K system ($z_A = z_B = 1$ as for Li^+-H^+; see also Tamaki [8]).

With this brief introduction to some characteristics of thermodynamics and pair correlations, we turn to a summary of results on dynamical structure. For a bare He^{++}-H^+ mixture on a rigid neutralizing background, McDonald *et al.* [9] used computer simulation techniques to investigate dynamical properties. Postogna and Tosi [10] have subsequently treated by largely analytical methods the dynamics of multi-component classical ionic plasmas in a polarizable background of electrons.

Their formulation was posed in the language of linear-response theory. They considered, in particular, the way the system responds to a set of weak external potentials $V_\alpha(\mathbf{q}, \omega)$ applied to the three components of the plasma. The matrix $\chi_{\alpha\beta}(\mathbf{q}, \omega)$ of density response functions relates the induced density changes to the external potentials:

$$\delta n_\alpha(\mathbf{q}, \omega) = \sum_\beta \chi_{\alpha\beta}(\mathbf{q}, \omega) V_\beta(\mathbf{q}, \omega). \tag{8}$$

As for a pure liquid metal (i.e. a two-component plasma), progress analytically is possible if the electron-ion interaction is assumed weak. In this case the inverse density response matrix of the screened mixture is given by

$$\chi^{-1}(q, \omega) = \begin{pmatrix} \hat{\chi}_{AA}^{-1}(q, \omega) & \hat{\chi}_{AB}^{-1}(q, \omega) & -v_A(q) \\ \hat{\chi}_{BA}^{-1}(q, \omega) & \hat{\chi}_{BB}^{-1}(q, \omega) & -v_B(q) \\ -v_A(q) & -v_B(q) & (4\pi e^2/q^2)[\varepsilon^{-1}(q, \omega) - 1]^{-1} \end{pmatrix}. \tag{9}$$

Here, $\hat{\chi}_{\alpha\beta}(q, \omega)$ for $\alpha, \beta = A$ and B denotes the density response functions of the bare ionic mixture, $v_\alpha(q)$ is the interaction between an electron and an ion of species α and $\varepsilon(q, \omega)$ is the dielectric function of the jellium model (for further details and for a calculation of the longitudinal mode frequencies of the three-component plasma, see Postogna and Tosi [10]).

For the pure liquid metal, eqn. (9) yields the relation

$$\chi(q, \omega) = \hat{\chi}(q, \omega)/[1 - \bar{v}(q, \omega)\hat{\chi}(q, \omega)] \tag{10}$$

between the response functions of the screened and of the bare ionic fluid. Here,

$$\bar{v}(q, \omega) = \frac{q^2 v^2(q)}{4\pi e^2}\left[\frac{1}{\varepsilon(q, \omega)} - 1\right]; \tag{11}$$

which is related to the effective ion–ion potential.

The generalization of the result (10) to the mixture involves the inversion of the matrix in eqn (9) to yield $\chi_{\alpha\beta}(q, \omega)$ for $\alpha, \beta = A$ and B. These quantities then relate to the dynamical partial structure factors through

$$\mathrm{Im}\chi_{\alpha\beta}(q,\omega) = -\frac{(n_\alpha n_\beta)^{1/2}}{2\hbar}[1 - \exp(-\hbar\,\omega)]S_{\alpha\beta}(q,\omega). \qquad (12)$$

Integrating $S_{\alpha\beta}(q, \omega)$ over all ω naturally leads back to the static partial structure factors.

In this connection it is relevant to comment on static structural differences between a fully ionized Li^{3+}-H^{+} plasma and the partially ionized Li^{+}-H^{+}: a matter discussed above in the long wavelength limit. In the strong coupling case corresponding to Γ large, the Li^{+} core radius becomes smaller than the radius corresponding to the excluded volume created by the strong Coulomb repulsion. Then Li^{+}-H^{+} becomes, in essence a one-component plasma, described by eqns. (10) and (11).

In summary, we have set down explicit screening conditions to be satisfied in Li-H plasmas in two different ionization states in eqns. (4) (7). A final two-component theory of such plasmas must embody these conditions precisely as they are consequences of the fact that long-range electric fields cannot exist in a conducting medium. We have then laid down a route, following the analytical procedure of Postogna and Tosi [10], by means of which the degree of ionization can be embodied in the dynamical structure. Should experimental data eventually become available on Li-H under metallic plasma conditions, numerical calculations should be practicable from the approach presented in this Letter.

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