

Concerning ion-ion interaction in metallic hydrogen

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We calculated the potential of the effective ion-ion interaction in metallic hydrogen. It is shown that the terms of third order in the electron-ion interaction play the principal role in the formation of the ion-ion interaction.

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The problem of metallic hydrogen (MH) has recently attracted much attention.¹¹⁻⁵¹ Analysis of the possible types of the structures of MH^{3,4)} has led to the conclusion that MH under pressure has peculiar tendencies. The question of the possible transition of hydrogen from the molecular phase into the liquid-metal phase can be solved only by direct calculation of the thermodynamic potential of the liquid phase and this, in turn, calls for knowledge of the potential of the interparticle interaction. In this paper we present the results of a calculation of the potential of the effective ion-ion interaction $\Phi(R)$ in MH.

As shown in Ref. 6, the potential of the effective ion-ion interaction in a metal has a direct component and an indirect component. The use of perturbation theory in the pseudopotential (PP) of the electron-ion interaction leads to a representation of $\Phi(R)$ in the form of the series

$$\Phi(R) = \Phi_2(R) + \Phi_3(R) + \dots, \quad (1)$$

where the subscript of $\Phi(R)$ shows the order in the PP. The thermodynamic properties of liquid alkali metals are satisfactorily described if only $\Phi_2(R)$ is taken into account in (1),¹⁷⁾ in which case $\Phi_2(R)$ takes the characteristic form of a Lennard-Jones potential with insignificant oscillations at large distances. For MH, the depth of the minimum of $\Phi_2(R)$ is very small.^{18,9)} It is therefore necessary to take into account the next terms of the perturbation-theory series. The contributions of terms in third order in the PP to the paired ion-ion interaction is obtained with the aid of the general theory¹⁶⁾ and can be represented in the form

$$\begin{aligned} \Phi_3(R) = & \frac{1}{4\pi^4} \int_0^\infty dq_1 \frac{w(q_1)}{\epsilon(q_1)} q_1 \int_0^\infty dq_2 \frac{w(q_2)}{\epsilon(q_2)} q_2 \int_{-1}^1 dz \frac{w(\kappa)}{\epsilon(\kappa)} \\ & \times \Lambda_0^{(3)}(q_1, q_2, \kappa) \left\{ \frac{\sin[(q_1 + q_2 z)R]}{(q_1 + q_2 z)R} + \frac{2\sin(q_1 R)}{q_1 R} \right\} \end{aligned} \quad (2)$$

where $u(q)$ is the form factor of the PP (for hydrogen $4\pi e^2/q^2$), $\kappa = (q_1^2 + q_2^2 + 2q_1 q_2 z)^{1/2}$, $A_0^{(3)}(q_1, q_2, \kappa)$, is an irreducible three-pole, and $\epsilon(q)$ is the effective dielectric constant (see Ref. 6).

Calculation of $\Phi(R)$ for MH by formula (1) with account taken of (2) was carried out with a computer. The polarization operator in $\epsilon(q)$ was chosen in the form proposed by Heldart and Vosko.⁽¹⁰⁾

Figure 1 shows the results of the calculations of the individual contributions made

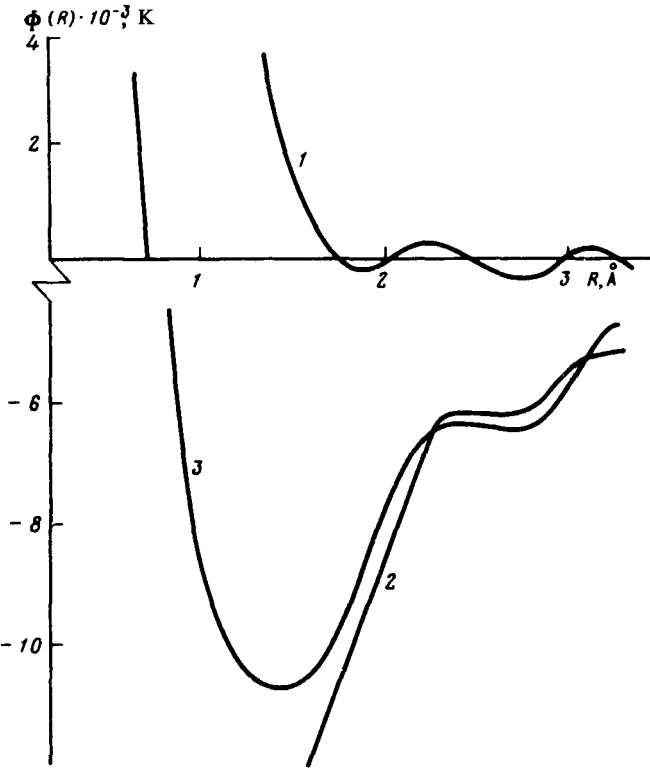


FIG. 1.

to $\Phi(R)$ at a density corresponding to $r_s = 1.45$ (r_s is the standard symbol for the radius of the sphere corresponding to the atomic volume, expressed in Bohr radii). Inclusion of all the second-order terms (curve 1) does not lead to formation of a potential well, in agreement with the calculations of Refs. 8 and 9, as well as with the results of Refs. 3 and 4. The contribution of the third-order term $\Phi_3(R)$ (curve 2) plays the decisive role in the determination of $\Phi(R)$ and leads to the appearance of a deep minimum on the resultant curve 3. We note that analogous calculations for alkali metals also lead to a considerable increase of the depth of the potential well on account of $\Phi_3(R)$ (~25%).

We investigated also the form of $\Phi(R)$ as a function of the pressure in the interval of r_s from 1.05 to 1.6. (If we use the equation of state obtained for MH in Ref. 5, then

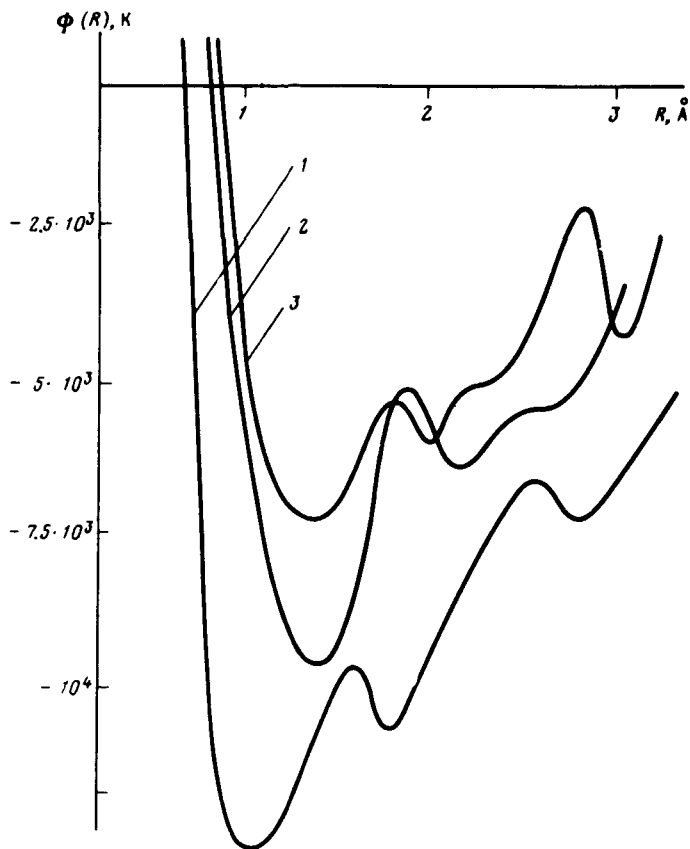


FIG. 2.

this interval corresponds to pressures from 0 to 10 Mbar). Curves 1, 2, and 3 on Fig. 2 pertain to $r_s = 1.6, 1.25,$ and $1.05,$ respectively. As follows from the presented figures, the change of the pressure leads to a change of the depth of the potential well. The decrease of the depth of the minimum with increasing pressure corresponds to an increase of the repulsion contribution to the energy from the direct ion-ion interaction, noted in Ref. 3. Next, in contrast to simple liquid metals, the $\Phi(R)$ curve exhibits several minima. The presence of these minima attests to a change occurring in the MH structure and accompanied by a realignment of the short-range order and by a change of the coordinate numbers, and reflects to a considerable degree the presence of different structures and the possibility of phase transitions in the crystalline phase.

Comparison of Figs. 1 and 2 also shows that the change of the pressure leads to alternation of more symmetrical and less symmetrical structures, as is the case for the solid phase.

Possessing data on $\Phi(R),$ we can calculate the thermodynamic properties of the MH in the liquid phase. This raises the problem of determining the radial distribution and the allowance for the irreducible three particle contributions to the thermodynamic characteristics.

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