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BULK MODULI OF LIQUID METALS BY THE HOMOGENEOUS DEFORMATION AND LONG WAVE METHODS

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The quantitative calculations of the bulk moduli of simple liquid metals continue to present difficulties. Hitherto, two types of methods have been used in the study of this problem: one is the homogeneous deformation (HD) method and the other is the long wave (LW) method. It is known that both methods are in principle equivalent [1]. But in actual calculations, where the perturbation expansion with the pseudopotential is used, the two methods present substantial differences at least in appearance. This fact is well recognized for solid metals and it is now established that the LW method within linear screening theory (i.e. second order theory in the pseudopotential) cannot explain the breakdown of the Cauchy relation [2] and produces too small bulk moduli of polyvalent metals [3]. On the other hand, one would expect the HD method within the same approximation to be more accurate because the leading contributions from the third and fourth order terms in the pseudopotential are effectively included in the course of taking density derivatives of pair interactions in this method [2].

One might therefore expect that the situation would be the same for liquid metals. In fact, Jones [4] roughly estimated the above mentioned extra contribution in the HD method and found it to be substantial, especially for polyvalent metals. On the contrary, Evans and Schirmacher [5] have shown that the LW method also produces an accurate long wavelength limit of the liquid structure factor, \( S(0) \), which is related to the bulk modulus \( B \) by \( S(0) = nk_BT/B \), \( n \) being the number density of atoms.

The purpose of this report is to examine this problem more systematically and to estimate more accurately the difference between the predictions of the two methods. The main conclusions of this investigation are as follows. (i) The contributions of the density dependence of the pair interaction (within linear screening theory), which is not accounted for in the LW method, is quite large for polyvalent metals. But the LW method happens to produce rather accurate bulk moduli of the simplest metals Na, Mg and Al. (ii) If we use appropriate pseudopotential parameters so as to reproduce average overall experimental liquid structure factors, the predictions of the LW method show good agreement with experimental data for almost all simple metals. This is as in the calculations by Evans and Schirmacher [5]. (iii) Even a sophisticated pseudopotential theory is still insufficient for the calculation of zeroth Fourier components and of the density dependence of (bare) pseudopotentials. This precludes exact calculations by the HD method, which should be more accurate in principle, in terms of such a pseudopotential and makes it difficult to decide on which method is practically advantageous.

Details of this report will be published...
elsewhere.


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