The Born-Green equation for liquid metals

Kumaravadivel, R.[a], Evans, R.[ab] and Greenwood, D.A.[a]

[a] H H Wills Physics Laboratory, Royal Fort, Tyndall Avenue, Bristol BS8 lTL, United Kingdom
[b] Institut für Theoretische Physik, Freie Universität, Berlin

Abstract

Conflicting reports have appeared in the literature concerning the usefulness of the Born-Green equation to determine effective interionic pair potentials in liquid metals from measured structure factors. To elucidate the problem, numerical investigations of the Born-Green equation have been made. These are based on recent structure factor data for sodium and potassium. Using the linearized simultaneous equation method of Waseda and Suzuki (1973), it is found that the equations in real space are ill conditioned. Hence a unique solution cannot be found numerically. However, in Fourier space unique solutions can be determined, but these solutions are temperature dependent. It is concluded that the temperature independent pair potentials for liquid metals which have been obtained from the Born-Green equation are not reliable.