MEAN SPHERICAL APPROXIMATION FOR A SYSTEM OF PARTICLES INTERACTING WITH DAMPED OSCILLATORY POTENTIAL

Viktor Urumov
Fakultet za Fizika, Gazi Baba, 91000 Skopje

An important characteristic of the interaction between the ions in a liquid metal is the presence of oscillations in the potential energy as a function of the interparticle distance /1/. In order to calculate the structure factor, different model potentials were proposed and by comparing them, one can notice a considerable distinction between them /2/. It is a characteristic feature of all the calculations performed so far that the interaction potential is cut-off at certain distance and no more than one oscillation is actually taken into account.

Although it has a number of deficiencies /3/ the so-called mean spherical approximation /MSA/ represents a frequently used approximation for different model potentials. The main argument in favour of the MSA is that it is exactly solvable in many cases, best known example being the Percus-Yevick equation for hard-core particles.

In the following we consider a system of particles interacting with the potential

$$V_i(r) = \begin{cases} +\infty & r<R \\ \dfrac{A e^{-\kappa r}\sin(lr+m)}{r} & r>R \end{cases} \qquad /a/$$

where A, κ, l, and m are parameters, r is the interparticle distance and R is the radius of the hard core of the particles. The above potential differs from the Friedel potential. The oscillations are damped by a factor $\frac{e^{-\kappa r}}{r}$ instead of $\frac{1}{r^3}$. The presence of an exponential damping may be expected because the Fermi surface in liquid metals is not as sharp as in solid metals /1/.

Accordingly we start from the equation of Ornstein and Zernike

$$h(r) = c(r) + \rho \int h(|\vec{r}-\vec{r}'|)\, c(|\vec{r}'|)\, d\vec{r}' \qquad /b/$$

where $h(r)=g(r)-1$ and $g(r)$ is the pair distribution function, $c(r)$ is the direct correlation function and ρ is the number

particle density. The equation /b/ is closed by the impenetrability condition $g(r)=0$ for $r<R$ and by the only assumption of MSA that for $r>R$ holds $c(r)=-\beta V(r)$ where β is the inverse temperature $\beta=\frac{1}{kT}$.

Following the standard procedure the initial problem is reduced to a system of six algebraic equations, which will be given elsewhere.

The following expression for the direct correlation function for $r<R$ is found

$$xc_0(x)=v_0+v_1x+v_2x^2+v_3x^4+v_4e^{\varkappa x}\cos\lambda x+v_5e^{\varkappa x}\sin\lambda x+v_6e^{-\varkappa x}\cos\lambda x+v_7e^{-\varkappa x}\sin\lambda x \quad /c/$$

where $x=\frac{r}{R}$, $\lambda=l.R$, $\varkappa=\kappa R$, $c_0(r)=c(r)+\beta V(r)$ and the coefficients v_i are given through the solution of the algebraic equations. These equations were solved numerically for some particular values of the parameters using the gradient and the Newton-Raphson methods.

Taking Fourier transform of /b/ and using the result /c/ and the MSA assumption it is easy to compute the structure factor. Comparing our results with the structure factor of Ashcroft and Lekner /4/ we conclude that the positions of the maxima and minima are unchanged. The amplitudes are changed only for low q /$q=k.R$ and k is the wave number/, the reduction of the height of the first maximum being most pronounced. The behaviour for large q is dominated by the hard-core repulsion and is almost unaffected by the presence of /a/. Presumably better agreement with experiment can be obtained if some soft repulsion is added and this can be tackled within MSA if we assume potential of the form

$$V=V_1+B\frac{e^{-nr}}{r}\quad,\ B>0$$

References

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