The Square-Well Model in
Random Phase Approximation:
Application to Structure of Liquid-Metal State

Arkadiy B. Finkel’shtein

Ural Federal University, Mira st. 19, 620002 Ekaterinburg, Russia

Copyright © 2014 Arkadiy B. Finkel’shtein. This is an open access article distributed under
the Creative Commons Attribution License, which permits unrestricted use, distribution, and
reproduction in any medium, provided the original work is properly cited.

Abstract

The structure factor of liquid sodium is calculated in the square-well (SW) model
within the random phase approximation at different values of the SW depth. It is
found that the increase of the absolute magnitude of the last not leads from some
moment to the improvement of the result.

Keywords: Square-well model, random phase approximation, structure factor,
liquid metal

In a general case the random phase approximation (RPA) for a classical fluid
is formulated as follows [1]:

\[ c_{\text{RPA}}(r) = c_0(r) - \beta \phi_1(r) \]

where \( c(r) \) is the direct correlation function, \( \phi(r) \) - pair interatomic potential,
\( \beta = (k_B T)^{-1} \), \( k_B \) - Boltzmann constant, \( T \) - absolute temperature, symbols “0”
and “1” are attributes of a reference system and perturbation, respectively.

For any hard-core (HC) \( \phi(r) \),

\[ \phi_{\text{HC}}(r) = \begin{cases} \infty, & r < \sigma \\ \phi(r), & r \geq \sigma \end{cases} \]

where \( \sigma \) is the HC diameter,

\[ c_{\text{RPA-\text{HC}}}(r) = c_{\text{HS}}(r) - \beta \phi(r) \]

Here, “HS” denotes the hard-sphere model which is described by the following \( \phi(r) \):
\[
\varphi_{HS}(r) = \begin{cases} 
\infty, & r < \sigma \\
0, & r \geq \sigma 
\end{cases}
\]  

(4)

For calculation of \( c_{HS}(r) \) the Wertheim-Thiele exact solution [2, 3] in the Percus-Yevick approximation [4] can be used.

The RPA structure factor, \( S_{RPA}(q) \), for the HC pair potential is

\[
S_{RPA-HC}(q) = \frac{1}{1 - \rho c_{HS}(q) + \beta \rho \phi(q)} ,
\]

(5)

where \( \rho \) is the mean atomic density, \( \phi(q) \) - Fourier transform of \( \phi(r) \).

In the case of the square-well (SW) pair potential,

\[
\varphi_{SW}(r) = \begin{cases} 
\infty, & r < \sigma \\
\epsilon, & \sigma \leq r < \lambda \sigma \\
0, & r \geq \lambda \sigma 
\end{cases}
\]  

(6)

where \( \epsilon \) and \( \lambda \) are parameters responsible for the SW depth and SW width, respectively, the structure factor is expressed as follows:

\[
S_{RPA-SW}(q) = \frac{1}{1 - \rho c_{HS}(q) + \beta \rho \phi_{SW}(q)} ,
\]

(7)

where

\[
\phi_{SW}(q) = \frac{4 \pi \epsilon}{q^3} [\sin(q \lambda \sigma) - \sin(q \sigma) - q \lambda \sigma \cos(q \lambda \sigma) + q \sigma \cos(q \sigma)] .
\]  

(8)

We apply (7) to calculate the structure factor of liquid Na at \( T=373K \) (Fig.1) with reasonable values of the SW parameters at experimental value of \( \rho \) [5].

![Fig.1](image-url)  

\( S_{RPA-SW}(q) \) of liquid sodium calculated at \( \lambda = 1.5 \) and \( \rho \sigma^3 = 0.8 \) in comparison with experiment [6] (solid line: \( \beta \epsilon = -1.2 \); dashed line: \( \beta \epsilon = -0.6 \)).
Results presented in Fig. 1. show that the structure factor obtained at $\beta \varepsilon = -0.6$ agrees better with experiment than the structure factor obtained at $\beta \varepsilon = -1.2$. This fact denotes that it is possible to find an optimal (between zero and infinity) SW depth for the description of a liquid metal structure.

References


Received: November 19, 2013