

## PSEUDOPOTENTIAL CALCULATION OF THE STRUCTURE AND THERMODYNAMICS OF LIQUID ALKALI METALS WITH A SQUARE-WELL MODEL AS A REFERENCE SYSTEM

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We investigate the applicability of a variational method with a new reference system (square-well model) to the description of the structure and thermodynamics of liquid metals. An expression for the system entropy for a one-component fluid is derived. The three parameters of the model (the hard-sphere diameter and the width and depth of the square well) are determined by the variational method using the local pseudopotential approximation. The approach is used for liquid Na and K, and the calculated results are compared with experiment. It is shown that the approach can provide a realistic description of the properties of liquid metals.

**Keywords:** liquid metal, reference system, pseudopotential, pair interatomic interaction, variational method, structure factor, thermodynamic properties.

### INTRODUCTION

A quantitative description of the properties of structurally disordered metals, including liquid metals, is one of the core problems in the theory of condensed matter. A successful resolution of this problem would require, first, a proper consideration of the electron structure of liquid metals and, second, an averaging over all possible atomic configurations. To carry out this averaging, one should be able to accurately calculate the correlation functions describing the structure of the liquid. We chose alkali metals (Na and K) as the object of our study because for these metals the pseudopotential method provides, in the second-order perturbation theory in the local approximation, a very accurate description of all interactions, i.e., electron–electron, electron–ion, and effective ion–ion interactions. As a result, for alkali metals, we can calculate numerically an almost exhaustive set of properties. Therefore, it is the alkali metals that are best suitable for studying the accuracy of various models of liquids.

The variational method [1] based on the Gibbs–Bogolyubov inequality is widely used in the calculation of the thermodynamic and structural properties of liquid metals, with the hard-sphere model (HS) [2–7] being mainly used as a reference system. However, there are attempts to use other reference systems, such as the one-component plasma (OCP) model [8], the charged hard spheres (CHS) model [9–11], and the hard-sphere Yukawa (HSY) model [12, 13].

In this paper we use a variational method with a new reference system that we proposed in [14], i.e., the square-well (SW) model.

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The SW potential is more realistic than the HS potential because, unlike the latter, it has an attractive part, due to which the potential energy of the model system is non-zero. Moreover, mathematically, the system is simple and convenient for use in various approximations of the theory of liquids. Therefore, there are a number of analytical and semi-analytical expressions for the SW model, which are obtained both in different versions of thermodynamic perturbation theory [15-18] and by using new mathematical methods for the solution of the Ornstein–Zernike (OZ) equation in the mean spherical approximation (MSA [19]) [20-22] and in the Percus-Yevick approximation (PY [23]) [24, 25]. In addition, we note here the semianalytical SW–MSA approach [26-28] that does not use the OZ equation in direct space and the work [29], in which Wertheim’s approach [30] is applied to the SW potential, resulting in an analytical PY solution for the SW model.

The most simple and convenient analytical expression for the structure factor of SW fluid [15] exists in the random phase approximation (RPA) [31, 32], which is why we chose this approximation to describe the SW of the reference system. The required SW–RPA expression for entropy was obtained in [14].

In contrast to the hard-sphere model, which has one free parameter (HS diameter), the SW model has three variational parameters: the diameter of the hard core of the interatomic potential and the depth and width of the square well. We investigated the behavior of free energy for different values of model parameters and found those areas of parameter that contain solutions. We chose those values of well width that lead to the most reasonable results. We found that these solutions lie on the boundary of admissible values of well width. The other two parameters were determined by minimizing the energy, and the square well proved to be a sufficiently wide, while its depth was very small. This situation is observed for both liquid metals under study. The results obtained for the structure and thermodynamic properties are in good agreement with experiment, which suggests that the proposed approach is quite promising. In addition, the model can be further developed and extended to multicomponent systems.

## THEORETICAL

In the general case, the pair potential with a hard core (HC),  $\varphi_{\text{HC}}(r)$ , can be written as

$$\varphi_{\text{HC}}(r) = \begin{cases} \infty, & r < \sigma \\ \phi(r), & r \geq \sigma \end{cases}, \quad (1)$$

where  $\sigma$  is the HC diameter.

The random phase approximation in the theory of simple liquids [15] suggests a combination of the mean spherical approximation (MSA) (proposed in [19] for systems with a potential given by (1)) with the representation of the direct correlation function  $c(r)$  inside the HC in the form of  $c_{\text{HS}}(r)$

$$c_{\text{RPA}}(r) = \begin{cases} c_{\text{HS}}(r), & r < \sigma \\ -\beta\phi(r), & r \geq \sigma \end{cases}, \quad (2)$$

where  $c_{\text{HS}}(r)$  is the direct correlation function of the hard sphere liquid (here we use the analytical form of  $c_{\text{HS}}(r)$  obtain in [30, 33] in the PY approximation).

Then the structure factor  $a(q)$  can be written as

$$a_{\text{RPA}}(q) = \frac{1}{1 - \rho c_{\text{HS}}(q) + \beta\rho\phi(q)}, \quad (3)$$

where  $c_{\text{HS}}(q)$  and  $\phi(q)$  are the Fourier images of  $c_{\text{HS}}(r)$  and  $\phi(r)$ , respectively;  $\rho$  is the mean atomic density;  $\beta = (k_{\text{B}}T)^{-1}$ ;  $k_{\text{B}}$  is the Boltzmann constant; and  $T$  is absolute temperature.

In the SW model, the pair potential has the form

$$\varphi_{\text{SW}}(r) = \begin{cases} \infty, & r < \sigma \\ \varepsilon, & \sigma \leq r < \lambda\sigma \\ 0, & r \geq \lambda\sigma \end{cases}, \quad (4)$$

where  $\varepsilon$  and  $\sigma(\lambda - 1)$  are the depth and widths of the well, respectively. Then,

$$\phi_{\text{SW}}(r) = \begin{cases} 0, & r < \sigma \\ \varepsilon, & \sigma \leq r < \lambda\sigma \\ 0, & r \geq \lambda\sigma \end{cases} \quad (5)$$

The Fourier image  $\phi_{\text{SW}}(q)$  is

$$\phi_{\text{SW}}(q) = 4\pi\varepsilon [\sin(\lambda x) - \sin(x) - \lambda x \cos(\lambda x) + x \cos(x)] / q^3, \quad (6)$$

where  $x = q\sigma$ .

The potential energy of SW fluid per atom  $U_{\text{SW}}$  is determined as follows:

$$U_{\text{SW}} = 2\pi\rho \int_0^{\infty} \phi_{\text{SW}}(r) g_{\text{SW}}(r) r^2 dr = 2\pi\rho \int_{\sigma}^{\lambda\sigma} \phi_{\text{SW}}(r) g_{\text{SW}}(r) r^2 dr, \quad (7)$$

where  $g(r)$  is the pair correlation function.

Using the known relationship between  $g(r)$  and  $a(q)$ , equation (7) can be transformed to

$$U_{\text{SW}} = \frac{1}{2} \rho \phi_{\text{SW}}(q=0) + \frac{1}{4\pi^2} \int_0^{\infty} [a_{\text{SW}}(q) - 1] \phi_{\text{SW}}(q) q^2 dq, \quad (8)$$

where

$$\phi_{\text{SW}}(q=0) = \frac{4}{3} \pi \sigma^3 \varepsilon (\lambda^3 - 1). \quad (9)$$

The entropy of SW fluid per atom  $S_{\text{SW}}$  consists of three contributions

$$S_{\text{SW}} = S_{\text{HS}} + \Delta S_{\text{SW}} = S_{\text{IG}} + \Delta S_{\text{HS}} + \Delta S_{\text{SW}}, \quad (10)$$

where  $S_{\text{HS}}$  is the entropy of HS fluid;  $S_{\text{IG}}$  is the entropy of the ideal gas, which in atomic units (au) is

$$S_{\text{IG}} = k_{\text{B}} \left[ \frac{5}{2} + \ln \left( \frac{1}{\rho} \left[ \frac{k_{\text{B}} T m}{2\pi} \right]^{\frac{3}{2}} \right) \right]; \quad (11)$$

$\Delta S_{\text{HS}}$  and  $\Delta S_{\text{SW}}$  are the contributions of HS repulsion and SW attraction; and  $m$  is the atomic mass.  $\Delta S_{\text{HS}}$  that was obtained from the compressibility equation was taken from [2]

$$\Delta S_{\text{HS}} = k_{\text{B}} \left[ \ln(1 - \eta) + \frac{3}{2} \left( 1 - \frac{1}{(1 - \eta)^2} \right) \right], \quad (12)$$

where  $\eta = (\pi\rho\sigma^3/6)$  is the packing density.

The contribution  $\Delta S_{\text{SW}}$  is derived from the well-known thermodynamic relationship

$$\left( \frac{\partial S}{\partial T} \right)_{\rho} = \frac{1}{T} \left( \frac{\partial E}{\partial T} \right)_{\rho}, \quad (13)$$

where  $E$  is the internal energy.

For SW fluid, equation (13) leads to

$$\left( \frac{\partial(\Delta S_{\text{SW}})}{\partial T} \right)_{\rho} = \frac{1}{T} \left( \frac{\partial U_{\text{SW}}}{\partial T} \right)_{\rho}. \quad (14)$$

Using relation (3) for SW potential and relation (8), we obtain

$$\left( \frac{\partial U_{\text{SW}}}{\partial T} \right)_{\rho}^{\text{RPA}} = \frac{\rho k_{\text{B}}}{4\pi^2} \int_0^{\infty} \frac{\phi_{\text{SW}}^2(q) q^2 dq}{[k_{\text{B}} T (1 - \rho c_{\text{HS}}(q)) + \rho \phi_{\text{SW}}(q)]^2}. \quad (15)$$

In deriving (15), we reversed differentiation and integration and considered the fact that the integrand depends on temperature only through the parameter  $\beta$ .

Integration leads to the following expression for  $\Delta S_{\text{SW}}$  in the RPA:

$$\Delta S_{\text{SW-RPA}} = \int \frac{dT}{T} \left( \frac{\partial U_{\text{SW}}}{\partial T} \right)_{\rho}^{\text{RPA}} = \frac{k_{\text{B}} \rho}{4\pi^2} \int_0^{\infty} \left[ -\frac{1}{\rho^2 \phi_{\text{SW}}^2(q)} \left( \ln \left| \frac{k_{\text{B}}}{a_{\text{SW-RPA}}(q)} \right| + (1 - \rho c_{\text{HS}}(q)) a_{\text{SW-RPA}}(q) \right) + C \right] \phi_{\text{SW}}^2(q) q^2 dq. \quad (16)$$

The integration constant  $C$  was determined from the condition  $\Delta S_{\text{SW-RPA}} = 0$  at  $\varepsilon = 0$  or  $\lambda = 1$  in order to obtain a correct limiting transition to the hard-sphere model

$$C = \frac{\ln |k_{\text{B}}(1 - \rho c_{\text{HS}}(q))| + 1}{\rho^2 \phi_{\text{SW}}^2(q)}. \quad (17)$$

Finally, we obtain

$$\Delta S_{\text{SW-RPA}} = \frac{k_{\text{B}}}{4\pi^2 \rho} \int_0^{\infty} q^2 \left( \ln |(1 - \rho c_{\text{HS}}(q)) a_{\text{SW-RPA}}(q)| - (1 - \rho c_{\text{HS}}(q)) a_{\text{SW-RPA}}(q) + 1 \right) dq. \quad (18)$$

The idea of the variational method with SW reference system is to minimize the following expression for free energy (per atom):

$$F_{\text{var}} = \frac{3}{2} k_{\text{B}} T + E_0 + E_1 + E_2 + E_3 - T(S_{\text{SW-RPA}} + S_e), \quad (19)$$

where  $E_0$  is the energy of the interacting electron gas;  $E_1$  is the contribution of the first order in the pseudopotential;  $E_2$  is the energy band structure, which is essentially the contribution of the second order in the pseudopotential;  $E_3$  is the Madelung energy; and  $S_e = zT \left( \frac{\pi k_{\text{B}}}{k_{\text{F}}} \right)^2$  is the contribution of the electron gas to the entropy (this contribution is sufficiently small).

The electron gas energy (au) is given by the expression

$$E_0 = \frac{3}{10} z k_{\text{F}}^2 + \frac{1}{2} S_e T - \frac{3}{4\pi} k_{\text{F}} + E_{\text{corr}}, \quad (20)$$

where  $z$  is valence and  $k_{\text{F}} = (3z\rho\pi^2)^{1/3}$  is the Fermi vector. The third term in (20) is the exchange energy of the electron gas, and the fourth term is its correlation energy. The value  $E_{\text{corr}}$  was taken in the Nozieres–Pines approximation [34] (au):

$$E_{\text{corr}} = z(-0.0575 + 0.0155 \ln r_{\text{S}}), \quad (21)$$

where  $r_{\text{S}} = (9\pi/4)^{1/3} k_{\text{F}}^{-1}$  is the electron radius.

It should be noted that relations (20) and (21) for the various contributions of electron gas to the energy, which were used in the numerical calculations, are sufficiently accurate for alkali metals.

The contributions that depend on the pseudopotential of the electron–ion interaction are defined as follows:

$$E_1 = z \lim_{q \rightarrow 0} \left( \omega(q) + \frac{4\pi\rho z}{q^2} \right), \quad (22)$$

$$E_2 = \frac{1}{2\pi^2 \rho} \int_0^{\infty} a_{\text{SW-RPA}}(q) F(q) q^2 dq, \quad (23)$$

where  $\omega(q) = \rho \int \omega(r) e^{-iqr} d^3r$  is the form factor of the unscreened electron–ion pseudopotential  $\omega(r)$  and  $F(q)$  is the characteristic function

$$F(q) = -\frac{q^2}{8\pi\rho} \omega^2(q) [(\varepsilon_{\text{H}}(q) - 1)^{-1} + (1 - f(q))]^{-1}. \quad (24)$$

Here  $\varepsilon_H(q)$  is the Hartree dielectric function:

$$\varepsilon_H(q) = 1 + \frac{1}{2\pi k_F x^2} \left( 1 + \frac{1-x^2}{2x} \ln \left| \frac{1+x}{1-x} \right| \right), \quad (25)$$

where  $x = q/2k_F$  and  $f(q)$  is the exchange–correlation function taken in the Vashishta–Singwi approximation [35] in a simple analytical form:

$$f(q) = A[1 - \exp(-Bq^2 / k_F^2)], \quad (26)$$

where  $A$  and  $B$  are parameters depending on the electron radius  $r_s$  and determined by interpolation from the table in [35].

To carry out the pseudopotential calculation, we need to choose the specific form of the pseudopotential. In this work, we used the Animalu–Heine model potential [36] in the local approximation [37]  $\omega_{LAH}(r)$ , whose form factor is:

$$\omega_{LAH}(q) = -\frac{4\pi\rho}{q^2} \left[ (z - A_M R_M) \cos(qR_M) + \frac{A_M R_M \sin(qR_M)}{qR_M} \right] \exp \left[ -0.03 \left( \frac{q}{2k_F} \right)^4 \right], \quad (27)$$

where  $A_M$  and  $R_M$  are the parameters of the pseudopotential. The choice of this potential is explained by the fact that it leads to a fairly accurate description of the properties of alkali metals in both solid and liquid states [3, 37].

The Madelung energy depends only on the structure of the ion subsystem (completely determined by the structure factor) and is given by

$$E_3 = \frac{z^2}{\pi} \int_0^\infty (a_{SW-RPA}(q) - 1) dq. \quad (28)$$

In the general case, the Helmholtz free energy can be minimized by three parameters: the diameter of the hard core and the depth and width of the square well.

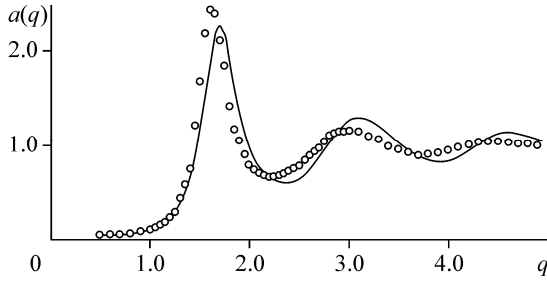
## RESULTS AND DISCUSSION

We applied the above formalism for the calculation of the structure factors and thermodynamic properties of liquid Na and K near the melting point at  $T = 373$  K. The input data are presented in Table 1. The pseudopotential parameters were taken from [37]; the experimental data on the average atomic density were taken from [38].

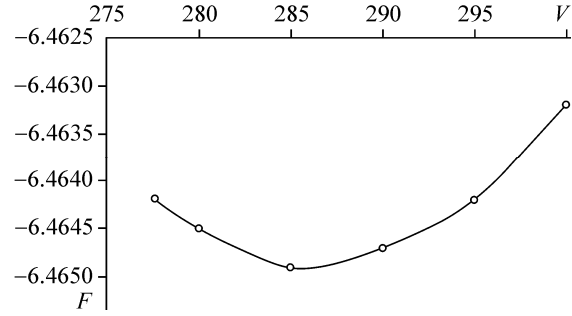
The solution in the SW–RPA approximation leads to an unphysical behavior of the structure factor for some sets of square well parameters, which does not allow for the minimization of free energy by all the three parameters over a wide range of their values. Therefore, we carried out the minimization by two parameters,  $\sigma$  and  $\varepsilon$ , at a fixed value of  $\lambda$ . We identified two areas of reasonable values of the parameter  $\lambda$ , one in the range 1.4–1.5 and the other in the range of 1.8–1.95. For these values the structure factor was positive. For other properties it was found that, in the first area, the thermodynamic properties (energy and entropy) have completely unreasonable values, which are significantly improved in the second area, with the best results being achieved for the maximum values of  $\lambda$  in the range. In this case the boundary where solutions are lost is very distinct. Therefore, we took the largest possible value of the parameter  $\lambda$  for each of the metals listed in Table 1. It is interesting to note that the values of the parameter  $\lambda$  are similar for both metals. For the remaining two parameters, the minimization was performed over a wide range of values, and the data obtained are also given in Table 1. Note that the values obtained for the diameter of the hard core are close to those obtained in the variational

**TABLE 1.** Input Data and Calculated Values of SW Parameters (au)

Metal	$R_M$	$A_M$	$\rho$	$\lambda$	$\sigma$	$\varepsilon$
Na	2.174	-0.2136	0.003602	1.926	6.2149	-0.000365
K	3.082	-0.1949	0.001885	1.933	7.6939	-0.000333



**Fig. 1.** Structure factor of liquid K near the melting points obtained using the SW-RPA reference system (solid line) as compared to the experimental data (circles).



**Fig. 2.** Dependence of free energy  $F$  (eV) on atomic volume  $V$  (au) for liquid Na near the melting point.

**TABLE 2.** Individual Contributions (eV) to the Internal Energy of Liquid Metals at  $T = 373$  K

Metal	$E_0$	$E_1$	$E_2$	$E_3$	$3/2k_B T$
Na	-2.21943	2.00965	-0.20543	-5.86522	0.04821
K	-2.17465	1.83565	-0.17297	-4.70499	0.04821

**TABLE 3.** Internal Energy  $E$  (eV) and Entropy  $S$  ( $k_B$  units) for Liquid Metals

Metal	$E$			$S/k_B$		
	SW-RPA	HS	Experiment	SW-RPA	HS	Experiment
Na	-6.232	-6.397	-6.149	7.22	7.49	7.79
K	-5.169	-5.119	-5.170	8.77	9.15	9.45

method with the hard-sphere reference system. Also note that the depth of the square well was very small in magnitude and negative in sign. Its numerical value is similar in the order of magnitude to the minimum of the pair potential calculated with the pseudopotential used in this study, which means that its value is reasonable. The width of the square well is greater than the width of the first minimum of the pair potential.

The structure factor of Na was calculated in [14], and Fig. 1 shows the results for the structure factor of liquid K in comparison with experimental data from [39]. In the region of the first peaks, the theoretical and experimental data are seen to be well consistent with each other.

The proposed procedure turned out to yield a deeper minimum of free energy than the hard-sphere model [14]. Figure 2 shows the calculated dependence of the free energy of liquid Na at  $T = 373$  K on volume per atom,  $V = 1/\rho$ . The minimum value corresponds to a density that differs from the experimental data by about 2%. It also confirms the good accuracy of the proposed model. Table 2 shows individual contributions to the total energy of the liquid metal in accordance with equation (19). The Madelung energy is seen to make the main contribution to the total energy. The zero- and first-order contributions in the pseudopotential largely cancel each other out, and the contribution of the second order is small. Finally, Table 3 shows calculated values of thermodynamic quantities, namely, the total internal energy  $E = 3k_B T/2 + E_0 + E_1 + E_2 + E_3$  and the total entropy  $S = S_{\text{SW-RPA}} + S_e$ , in comparison with experimental data [40] and the data obtained using a hard-sphere model as a reference system. The consistency with the experimental data is quite reasonable.

## CONCLUSIONS

Our studies have shown the fundamental possibility of using the square-well model as a reference system in the variational method of the thermodynamic perturbation theory.

Better results may be obtained by using more accurate expressions parameterized on the basis of computer experiments (see, e.g., [41-45]) in the description of the HS model instead of those derived in the PY approximation. However, the most significant progress in the development of the variational method with SW reference system can be achieved by avoiding RPA altogether and using more sophisticated approaches (see, e.g., [16-18, 20-22, 24-29]).

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