# STRUCTURE OF LIQUID ALKALINE EARTH METALS AND METAL ALLOYS USING A NEW TRANSFERABLE LOCAL PSEUDOPOTENTIAL

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In this work, we have obtained the structural properties of liquid Ca, Sr and Ba near their melting points using the thermodynamically self consistent liquid state theory, the variational modified hypernetted chain (VMHNC) approximation with the effective pair potentials which are derived from the second order perturbation theory using the recently proposed transferable electron-ion potential of Fiolhais and co-workers. One has been noted that this potential is non realistic for the alkaline earths (Ca, Sr, Ba) because of the strongly nonlocal character. In this work, it has been shown that the computed structure factors and pair distribution functions near their melting points are in good agreement with experimental data. It has been also applied to the liquid alloys to predict the pair interactions and the partial structure factors by taking Li-Ba as a model alloy. The structural properties of Li-Ba alloys are presented for different concentrations by comparing with experimental data.

## 1. Introduction

The present paper is devoted to the theoretical study of some structural properties of simple liquid alkaline earth metals and metal alloys. From a theoretical of view, the study of simple metals is closely related to pseudopotentials [1]. Structure of the simple metals in their liquid state are well described using the effective inter-ionic interaction derived from the pseudopotential theory [1-3]. In principle the pseudopotentail can be of local or non-local character. Although some researchers have been preferred non-local pseudopotentials, it has been noted that, in some cases the local model pseudopotentials describe the some liquid state properties even better than those of norm conserving non-local ones [4].

In this work we have concerned with a recently proposed local model pseudopotential of Folhais *et al.* [5], whose parameters are fitted on the thermodynamic properties of the solid state. Two versions of this potential have been considered with individual and universal choices for parameters. It has been obtained that a second-order perturbative calculation with these pseudopotentials are in good agreement with the predicted physical properties in the solid state and the individual pseudopotential is better choice for each sixteen simple metal in generally [5]. It has been applied to finite systems for dimers, clusters and metallic slabs [6-7] and noted that its transferability is high for ten metals (K, Rb, Cs, Mg, Al, Ga, In, Tl, Sn and Pb), poor for Li, Be, Ca, Sr and Ba [6]. All these works doesn't prove this pseudopotential is applicable to liquids. It is the main aim of the presented paper.

In one of our previous work [8], it has been shown that the individual version of this model potential is transferable for liquid alkaline and alkaline earth metals using very accurate integral

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equation of liquids, the variational modified hypernetted chain (VMHNC) approximation [9-12]. Boulahbak *et al.* [13] and Tammar *et al.* [14] have also shown the universal version of the local pseudopotential of Fiolhais *et al.* using the soft-core mean spherical approximation (SMSA) is transferable for simple liquid alkaline metals, Li, Na, K, Rb, Cs but not alkaline earths and polyvalent ones. Related to this, we have also calculated the structure factor S(q) for liquid polyvalent simple metals using the individual choice of Fiolhais' potential with VMHNC integral equation theory disagrees with experimental data [15]. Recently we have presented the results for liquids Fe, Co and Ni, using the universal parameters which has been obtained with the proposed parameterization in that work [16]. According to our knowledge, this model potential has not been extended to liquid binary aloys. This is the second aim of this work. In present work, we took interest liquid Ca, Sr, Ba and Li-Ba alloys for which some authors have the successful results for their structural and thermodynamic properties using the Neutral Pseudo Atom (NPA) method potentials [11, 12]. We show that both the individual and universal choices of Fiolhais' potential predicts more reasonable structural properties for liquid Ca, Sr and Ba than NPA and others. Both version of this potential can be extended successfuly, to liquid binary alkaline alloys, such as liquid Na-K alloys [17]. However its transferability is a cause of concern for the charge transferred alloys, such as Li-Ba liquid alloys in the zero alloy case.

The layout of the paper is as follows. In section 2, we outline the theoretical basis of our work. The calculated effective pair potentials and the structure factors for liquid Ca, Sr and Ba are presented in section 3. The structural properties of liquid Li-Ba alloys at different concentrations are also presented by comparing with experiment in the same section, together with a brief discussion. Finally, in Section 4, we sum up and briefly comment on the results of our work.

## 2. Theory

### 2.1 Effective pair potentials

The effective inter-atomic pair potential in simple metals $\phi(r)$ is based on the use of pseudopotentials to describe the interaction between an ion and a second ion and its screening cloud of electrons from second order pseudopotentail perturbation theory , obtained by,

$$\phi(r) = \frac{Z_v^2}{r} + \phi_{ind}(r) \, , \tag{1}$$

where $Z_v$ for the effective number of valence electrons per atom and here Fourier transform (FT) of the indirect part is given by

$$\tilde{\phi}_{ind}(q) = \chi(q)\left|\tilde{v}(q)\right|^2 \, , \tag{2}$$

where $\tilde{v}(q)$ is the pseudopotential local form factor and $\chi(q)$ is the response function of the electron gas. The effects of exchange and correlation between the electrons are accounted for by the introduction of a local field factor G(q) in the response function as

$$\chi(q) = \frac{\chi^0(q)}{1 - \frac{4\pi}{q^2}\left[1 - G(q)\right]\chi^0(q)} \tag{3}$$

where $\chi^0(q)$ is the response function of a non-interacting electron gas. Here we employ the well known local field corrections of the Ichimaru-Utsumi (IU) [18] and the local density approximation (LDA) version of the local-field function G(q) with the correlation energy of Vosko - Wilk and Nussair (VWN) [19]. In the present work, we use the recent local pseudopotential proposed by

Fiolhais et al.[5,6]. This model pseudopotential has the core repulsion represented by an exponential factor, so called evanescent core (EC) pseudopotential. An analytic expression for the form factor of this pseudopotential in Fourier space:

$$\tilde{v}(q) = 4\pi Z_v R^2 \left[ -\frac{1}{(qR)^2} + \frac{1}{(qR)^2 + \alpha^2} + \frac{2\alpha\beta}{\left[(qR)^2 + \alpha^2\right]^2} + \frac{2A}{\left[(qR)^2 + 1\right]^2} \right] \tag{4}$$

where R is the core decay length, $\beta$ and A parameters are given in terms of $\alpha$ namely,

$$\beta = \frac{\alpha^3 - 2\alpha}{4(\alpha^2 - 1)}, \qquad A = \frac{\alpha^4}{4(\alpha^2 - 1)} \tag{5}$$

The values $\alpha$ and R can be obtained from the equilibrium condition of the solid state using the LDA [5,6]. For this reason this model potential has the advantage to be free of adjustable parameters. Fiolhais and co-workers have given the individual and universal pseudopotential parameters, EC(I) and EC(U) respectively, for sixteen simple metals in Ref. [5]. But the parameters R and $\alpha$ of the EC(U) pseudopotential for several values of the average valence electron density $r_S$ and valence Z are given for a table in Ref. [7]. The resulting effective pair potential for liquid alkaline earth metals contains three parameters, R, $\alpha$ and $Z_v$.

A simple liquid metallic alloy, $A_x B_{1-x}$, may be regarded as an assembly of A-type and B-type bare ions with charges $Z_v^A$ and $Z_v^B$ respectively, where $x$ is the concentration of the A-type component. Moreover, the ions attract the valence electrons which pile up around them, thus screening the ionic potentials and leading to effective interactions between the ions.

Now, once the A-type and B-type effective local pseudopotentials, $v_{ps}^A(q), v_{ps}^B(q)$ have been obtained, application of standard second-order perturbation pseudopotential theory leads to the effective interionic pair potentials, $\phi_{ij}(r)$, ( i, j = A, B) given by

$$\phi_{ij}(r) = \frac{Z_v^i Z_v^j}{r} + \phi_{ps}^{ij}(r) \tag{6}$$

where the Fourier transform of $\phi_{ps}^{ij}(r)$ is given as

$$\phi_{ps}^{ij}(q) = \chi(q) \tilde{v}_{ps}^i(q) \tilde{v}_{ps}^j(q) \tag{7}$$

Here , $\chi(q)$ is the response function of the electron gas as described above.

### 2.2 The VMHNC theory of liquids

With the effective pair potential known, integral equations are able to provide us the liquid structure for metals. In our structural calculations, one of the integral equation theory which has shown to be very reliable theory of liquids VMHNC has been carried out [9,10]. Like most liquid state theories the VMHNC solves the Ornstein - Zernike(OZ) equation :

$$h(r) = c(r) + \rho \int d\vec{r}' h(|\vec{r} - \vec{r}'|) c(\vec{r}') \tag{8}$$

which relates the direct correlation function c(r), in terms of the total correlation function, h(r)=g(r)-1 to the pair distribution g(r), within an approximate closure given as

$$c(r) = h(r) - \ln\left[g(r)\exp(\beta\phi(r) + B(r)\right] \tag{9}$$

where $\beta = (k_B T)^{-1}$, and $B(r)$ is the bridge function, $\rho$ is the ionic number density. In this work we use the analytic solution of the Percus-Yevick (PY) equation for hard spheres, $B(r) = B_{PY}(r, \eta)$ [9], where the packing fraction $\eta = \eta(\beta, \rho)$ is variationally determined for each termodynamic state by minimizing the VMHNC configurational free energy $f^{VMHNC}(\beta, \rho, \eta)$ at a temperature T, as

$$\frac{\partial f^{VMHNC}(\beta, \rho, \eta)}{\partial \eta} = 0 \tag{10}$$

The Ornstein-Zernike equation, which for a homogeneous, isotropic, binary system reads (i, j =1, 2)

$$h_{ij}(r) = c_{ij}(r) + \sum_{l=1}^{2} \rho_l h_{il}(r) * c_{lj}(r) \tag{11}$$

which defines the partial direct correlation functions, $c_{ij}(r)$, in terms of the total correlation functions $h_{ij}(r) = g_{ij}(r) - 1$, where $g_{ij}(r)$ denote the partial pair distribution functions and $\rho_l$ denote the partial ionic number densities. Now, Eq.(11) is supplemented by the exact closure relation

$$c_{ij}(r) = h_{ij}(r) - \ln\left[g_{ij}(r)e^{\beta\phi_{ij}(r) + B_{ij}(r)}\right] \tag{12}$$

where $\phi_{ij}(r)$ are the interatomic pair potentials and the $B_{ij}(r)$ denotes the PY bridge functions for binary system.

Formally the generalization of liquid state from monatomic to binary fluids, we have now a set of three coupled integral equations relating the partial pair distribution functions $g_{ij}(r)$ to the pair potentials $\phi_{ij}(r)$. The partial pair distribution functions are related to the partial structure factors $S_{ij}(r)$ by

$$g_{ij}(r) = 1 + \frac{1}{8\pi^3(\rho_i\rho_j)^{1/2}} \int (S_{ij}(q) - \delta_{ij})\exp(-iqr)dq \tag{13}$$

For binary liquid metal alloys we have carried out the VMHNC integral equation theory in which was extended by Gonzalez $et$ $al.$ [6], so as to minimize the configurational Helmholtz free energy functional $f^{VMHNC}(\beta, \rho, x_1, \eta_\alpha)$ by the variational condition

$$\frac{\partial f^{VMHNC}(\beta, \rho, x_{1,}\eta_\alpha)}{\partial \eta_k} = 0 \quad , \text{k=1,2,...,m} \tag{14}$$

for the m component system. We have chosen $\eta$ for the actual packing fraction of the system.

## 3. Results and discussion

### 3.1 Simple liquid metals

Firstly, we have presented the structural properties of liquid alkaline earth metals, Ca, Sr and Ba using the VMHNC liquid state theory with recently proposed Fiolhais' potentials. In Table 1, we

show the corresponding thermodynamic states for which the present study has been carried out. The input temperatures and corresponding number densities $\rho$ are taken from Waseda [15]. As already indicated in the preceding section, the calculation of the liquid structure requires, as a first step, the calculation of the interatomic pair potentials. In this work, the interatomic pair potentials of the pure liquid metals have been derived within the frame work of second order perturbation theory and using both the universal and individual Fiolhais' model potential for the electron-ion interaction. The universal Fiolhais' potential parameters $\alpha_U$ , $R_U$ obtained by the parameterisation procedure given in Ref. [16] are shown in Table 1. The individual Fiolhais' potential parameters $\alpha_I$ , $R_I$ taken from Ref. [5] are given in the same table.

Table 1. Thermodynamics states ($\rho$ ,T), pseudopotential parameters $\alpha$ and R, the Ashcroft core radius $R_c$ .

| Metal | T(K) | $Z_v$ | $\rho$(atoms/$\mathring{A}^3$) | $R_c$(a.u.) | $\alpha_I$ (a.u.) | $R_I$ (a.u.) | $\alpha_U$ (a.u.) | $R_U$ (a.u.) |
|-------|------|-------|------|------|------|------|------|------|
| Ca | 1123 | 2 | 0.0206 | 1.84 | 3.264 | 0.540 | 3.122 | 0.565 |
| Sr | 1053 | 2 | 0.0164 | 2.08 | 3.176 | 0.614 | 3.028 | 0.635 |
| Ba | 1003 | 2 | 0.0146 | 2.10 | 3.113 | 0.651 | 2.980 | 0.670 |

The calculated interatomic pair potentials for liquids Ca and Sr are plotted in Fig. 1a and Fig. 1b, respectively. The Fiolhais' effective pair potentials for Ca, which has been obtained by the individual parameters using different local-filed corrections are shown in Fig. 1a. The universal Fiolhais' pair potentials for liquid Sr obtained by using different screening functions are illustrated in Fig. 1b. For comparison, our Fiolhais' pair potentials are shared with the NPA pair potentials and pair potentials obtained by using the Ashcroft model [20] with IU approximation where the corresponding $R_c$ values are taken from Ref. [11]. We have also included in Fig. 1a that the interatomic pair potentials obtained by Moriarty through the use of the generalised pseudopotential perturbation theory (GPPT) [21]. It appears in Fig. 1b that the VWN-LDA local-field function gives rise to a deep potential well and small Friedel oscillations, while the IU yields a shallow well.
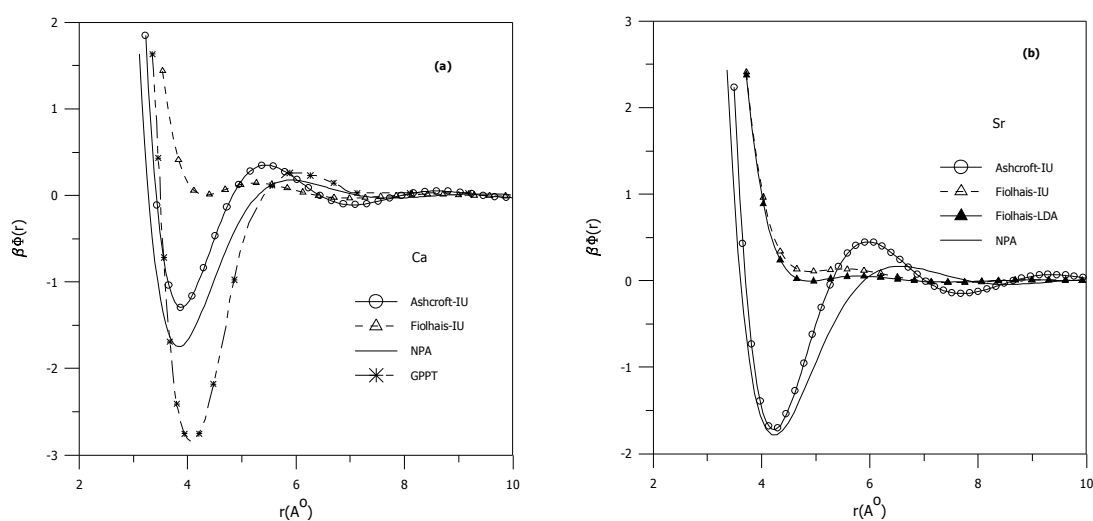


Fig. 1. Effective pair potentials for (a) Ca and (b) Sr.

The comparison between the pair potentials, those obtained by others and the present ones has shown that Fiolhais' potentials are always shallower and their positions shifted towards larger values of r. It is also clearly seen in Fig. 1a that the location of the first minimum of Fiolhais' potential for Ca is close to the GPPT pair potential. However we have noted that the calculated both version of Fiolhais' pair potentials using both LDA and IU screening functions show rather different trends with the NPA pair potentials. As we go down in the column, the Fiolhais potential becomes softer, but the width increases, and the position of the principal minimum is displaced to larger values of r.

These effective potentials are used as input data in our structural calculations. For pure liquid metals, we have solved the O-Z equation (8) with the closure relation (9) using Zerah's algorithm [22]. Fig. 2 represents our calculated static structure factors S(q) using the individual Fiolhais' potentials with the LDA screening, along with the corresponding experimental results of Waseda [15] and comparison with the VMHNC results using the NPA pair potentials. We find a good agreement between our calculated S(q)'s and experimental data; the positions and amplitudes of the oscillations are well reproduced. The LDA and IU screenings with both version of Fiolhais' model potential yield very similar results, both in good agreement with the experimental data though the first peak is slightly overestimated, it is also the case for the other alkali metals [8]. The VMHNC results using NPA interatomic pair potentials with an overestimated first peak exhibit a good agreement with the experimental results. This discrepancy between the VMHNC results and experimental data were discussed in Ref. [11]. We also find that the oscillations in our calculated S(q) die out more rapidly than in the experimental data. It is suggesting too soft a repulsive potential.
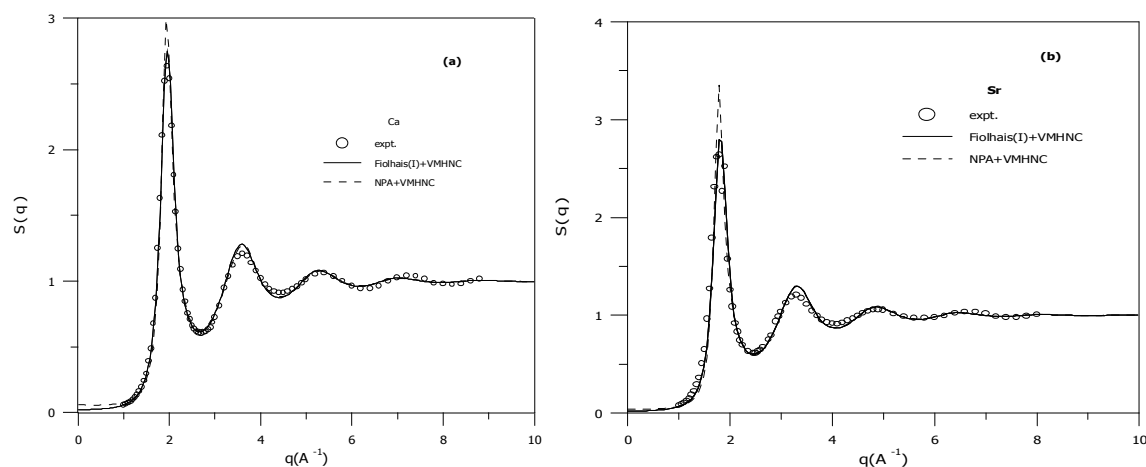


Fig. 2. Liquid static structure factors for (a) Ca and (b) Sr.

Our calculated S(q)'s in the low-q region fit very well experiment. The calculated values of S(0) are 0.022, 0.020, 0.020 for Ca, Sr and Ba, respectively comparing with the experimental values of 0.031, 0.032 and 0.035.

### 3.2 Liquid binary alloys

As described in the preceding section, we have applied the Fiolhais' model potential to study the structural features of the liquid binary Li-Ba alloys. In Table 2, we show the specific thermodynamic states for which the present study has been carried out. The total ionic number densities used in the calculations have been from the experimental results of Ruppersberg and coworkers [24,25]. Their measurements at T = 575 K and Ba concentrations $x_{Ba} = 0.12$ and 0.3 (the latter corresponding to the zero alloy) show a small tendency to homocoordination.

Table 2. Input data for liquid $Li_xBa_{1-x}$ alloys.

| Substance | $Z_{eff}$ | $\rho(atoms/Å^3)$ |
|-----------|-----------|-------------------|
| Li | 1 | 0.04344 |
| Ba | 2 | 0.01520 |
| $Li_{70}Ba_{30}$ | 1.30 | 0.02809 |
| $Li_{88}Ba_{12}$ | 1.12 | 0.03560 |

We have noted that the structure of both pure liquids Li and Ba near their melting points are well described with the individual version of Fiolhais' pair potentials obtained by using the LDA screening. The pseudopotential parameters taken from Ref. [5] are used in our liquid Li-Ba alloy calculations. The static structure factors for liquid Ba near the melting point are shown in Fig. 3. For $Li_xBa_{1-x}$ liquid alloys, partial structure factors have been calculated by using the interatomic pair potentials and Ashcroft - Langreth (AL) [26] and Bhatia - Thornton (BT) [27] descriptions with VMHNC. In this paper we present results for the AL partial structure factors $S_{ij}(q)$ (i, j = 1, 2) of the liquid alloy $Li_{70}Ba_{30}$ and the BT structure factors $S_{\alpha\beta}(q)$ ($\alpha, \beta = N, C$) of the liquid alloy $Li_{88}Ba_{12}$.
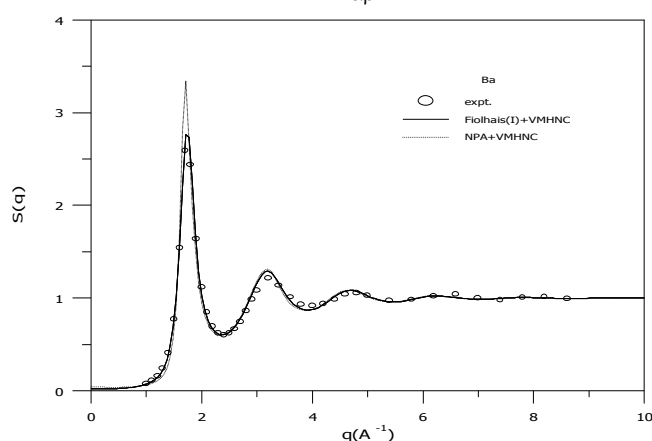


Fig. 3. Static structure factors for liquid Ba.

Fig. 4 shows the obtained Fiolhais' interatomic pair potentials $\phi_{ij}(r)$ for the liquid $Li_{70}Ba_{30}$ alloy in comparing with the NPA potentials [28]. It is observed that the trends in the changes shown by the $\phi_{ij}(r)$, are different in the NPA method.
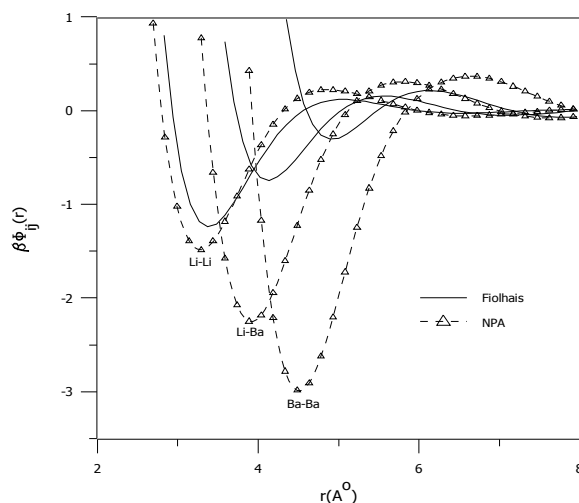


Fig. 4. Interatomic pair potentials, $\phi_{ij}(r)$, for the $Li_{70}Ba_{30}$ liquid alloy.

Fig. 5 and Fig. 6 show the AL partial structure factors of $S_{LiLi}(q)$ and $S_{LiBa}(q)$ in the $Li_{70}Ba_{30}$ and $Li_{88}Ba_{12}$ liquid alloys, respectively. We have also included the VMHNC results with NPA potentials and the hard-sphere (HS) results for the AL partial structure factors calculated with Percus-Yevick approximation using the parameters given in Ref. [25]; a corresponding program is given in Waseda's book [15]. In general, there is overall good agreement between the Fiolhais' $S_{LiLi}(q)$'s and others, except in the small-q region. The Fiolhais' based results of $S_{LiLi}(q)$ show a small phase shift for the region $q \geq q_{peak}$ though. $S_{LiLi}(q)$'s for the NPA and PY-HS are almost identical.



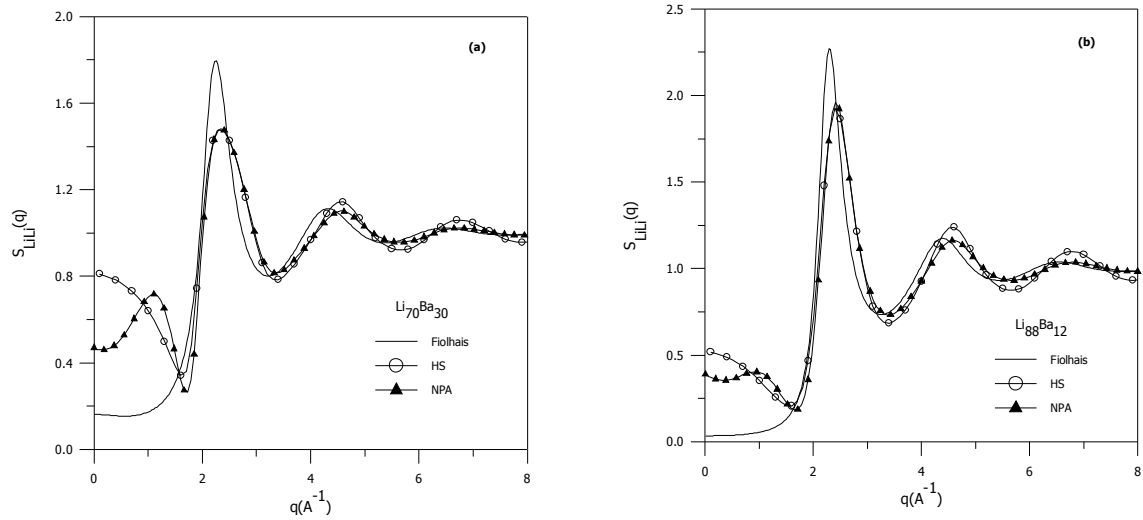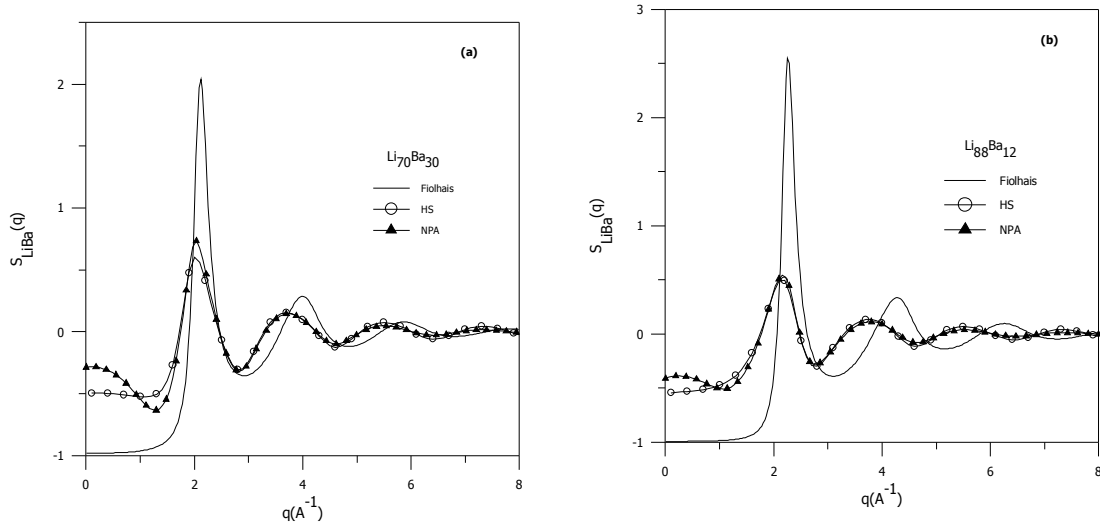Fig. 5. The AL partial structure factors $S_{LiLi}(q)$ in the liquid $Li_x Ba_{1-x}$ alloy.



Fig. 6. The AL partial structure factors $S_{LiBa}(q)$ in the liquid $Li_x Ba_{1-x}$ alloy.

In the case of $S_{LiBa}(q)$, the discrepancy between the Fiolhais' results and those obtained by others becomes rather marked. However the positions and amplitudes of the oscillations are almost identical for the NPA and PY-HS based results for $S_{LiBa}(q)$. We must point out that the discrepancies shown by these three theoretical results are in the small q region. The calculated number-concentration BT partial structure factor $S_{NC}(q)$ for the $Li_{88}Ba_{12}$ liquid alloy are shown in Fig. 7 in

comparison with the VMHNC results with the NPA potentials and the PY-HS results. It can be seen in Fig. 7 that the NPA based VMHNC results are almost identical with those obtained by the PY equation for binary mixtures of hard spheres [15]. The curve of the calculated $S_{NC}(q)$ is similar to others but rather different with in the depth and positions of oscillations

As indicated above, the composition $Li_{70}Ba_{30}$ is called the zero alloy for the $Li_x Ba_{1-x}$ liquid alloy. It yields the total structure factor $S(q) = S_{CC}(q)/c_1 c_2$ where $S_{CC}(q)$ is the concentration-concentration partial structure factors defined by BT. The total structure factors for the $Li_{70}Ba_{30}$ liquid alloy calculated with Fiolhais potentials using the VMHNC theory are given in Fig. 8. For comparison, we have also included the NPA and HS-PY based results and experiment.
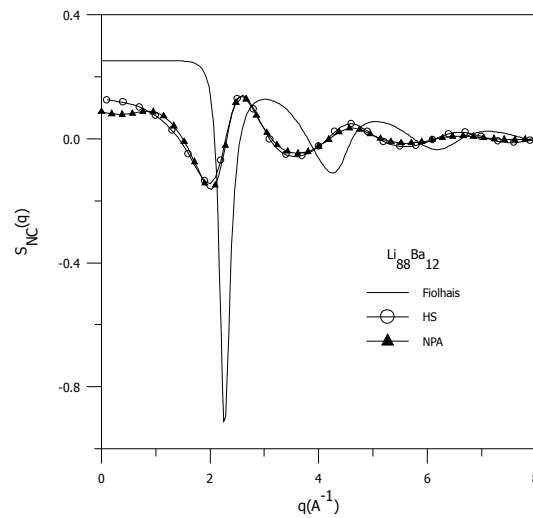


Fig. 7. The $S_{NC}(q)$ partial structure factors in the liquid $Li_x Ba_{1-x}$ alloy liquid alloy.
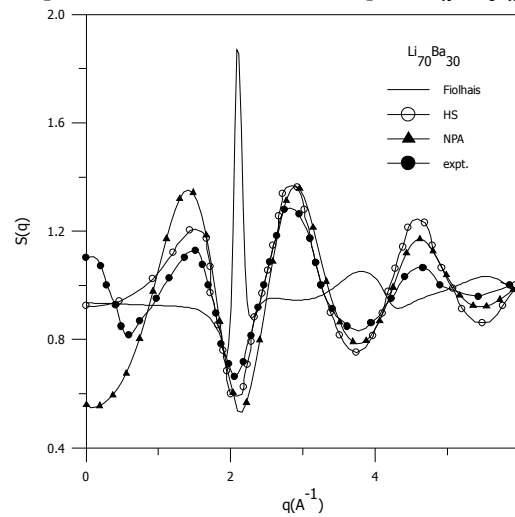


Fig. 8. The total structure factor $S(q) = S_{CC}(q)/c_1 c_2$ at the zero alloy case.

It is clear in Fig. 8 that both NPA and PY-HS theoretical results exhibit similar trends with experiment, except in small q region when the Fiolhais based results show different trends.

## 4. Conclusions

In the present work, we have predicted more reasonable structural results for liquid Ca, Sr and Ba using the VMHNC liquid state theory with the both version of Fiolhais' pair potentials. We conclude that the Fiolhais' potentials can be transferred to liquid state for Ca, Sr and Ba. We have extended the Fiolhais' model potential to the case of liquid binary alloys and we have applied it to study the structural properties of the $Li_x Ba_{1-x}$ liquid alloy at T=575 K. The combination of the Fiolhais' potentials to obtain the interatomic pair potentials with the VMHNC theory of liquids to obtain the liquid static structure, gives rise to a whole theory. The present formulation for liquid metallic alloy, $A_x B_{1-x}$ starts from the electron-ion potentials with screening functions and finally to the interatomic pair potentials in the alloy. The obtained interatomic pair potentials show rather different trends than those obtained by using the NPA potentials. However, the obtained results for the liquid partial structure factors of $S_{LiLi}(q)$ in both composition of the $Li_x Ba_{1-x}$ liquid alloy show a good agreement with others, except in the small q region. The results based on Fiolhais' potentials for $S_{BaBa}(q)$ structure factors of both composition are rather different. We note that $x_{Li}$ is increased, the differences between the NPA and PY-HS results of AL partial structure factors is also slightly decreased. We consider that the reason of these discrepancies is the charge transfer effects in $Li_x Ba_{1-x}$ liquid alloys. One of us has reported in elsewhere [12], the discrepancies between NPA and experiment in small q region were reduced when the charge transferred to Li.

However, this does not imply that the use of second order perturbation theory along the Fiolhais' potential will not be enough theoretical tool in order to explain the observed structural properties of liquid binary alloys. We believe that the Li-Ba alloy is a cause of concern. On the other hand, we have applied the whole presented theory to the $Na_x K_{1-x}$ liquid alloy at T=373K. We will present these results in near future.

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