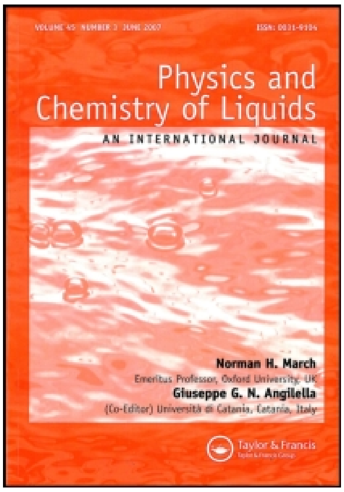

**Physics and Chemistry of Liquids**
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713646857

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**To cite this Article** Bretonnet, J. L. and Khanna, K. N.(1986) 'Non-Locality Effects of the Model Potential on the One-Component Plasma Structure Factor', Physics and Chemistry of Liquids, 15: 4, 265 — 269
**To link to this Article: DOI:** 10.1080/00319108608078488
**URL:** http://dx.doi.org/10.1080/00319108608078488

*Phys. Chem. Liq.*, 1986, Vol. 15, pp. 265–270
0031-9104/86/1504-0265$18.50/0

Printed in the United Kingdom

# Non-Locality Effects of the Model Potential on the One-Component Plasma Structure Factor

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*(Received July 9, 1985)*

We demonstrate that non-locality of the model potential plays a dominant role in the determination of the structure factor of alkali metals in the OCP model. Shaw's non local model potential combined with an analytic form of the direct correlation function in the Baus and Hansen scheme is found accurate to determine the structure factor of alkali metals up to the first peak.

During the last few years several attempts were made to develop an analytical function for the structure factor in the one component classical plasma reference system. Though the numerical experiments of the Monte-Carlo simulation[1,2,3] are available, it has not yet been possible to describe correctly the OCP structure factor analytically which is as convenient for the calculations as for hard sphere system. Charturvedi *et al.*[4] obtained an approximate agreement between the calculated and the measured value of the first peak height in the structure factor $S(q)$. Evans and Sluckin[5] have calculated $S(q)$ in the long-wavelength limit by using the correlation function suggested by Baus and Hansen.[6]

In the present communication, we analyse an analytic form for the structure factor of the OCP model by using the random phase approximation (RPA) to take into account the screening electron gas. The assumption is made that the ionic liquid and the electron gas are weakly coupled to each other through a pseudopotential. In order to show the role played by the non locality, we use a local model potential of Ashcroft[7] and a non local model potential of Shaw.[8]

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The bare OCP system, characterized by dimensionless parameter $\Gamma = \beta Z^2 e^2/a$ where $a$ is the ion sphere radius $a = (4\pi\rho/3)^{-1/3}$, is generally a crude approximation. The system can be modified by allowing the conduction electrons to screen the structure of OCP reference system in the RPA. To our knowledge, RPA is a simple but effective approach to describe the structure factor of alkali metals in OCP reference system. As is well known, the structure factor in the random phase approximation can readily be expressed as

$$S(q) = \frac{1}{1 - \rho[C_{\mathrm{OCP}}(q) - \beta u_{\mathrm{SC}}(q)]} \tag{1}$$

here $C_{\mathrm{OCP}}(q)$ is the Fourier transform of the direct correlation function expressed by Baus and Hansen[6] as

$$C_{\mathrm{OCP}}(q) = -\frac{4\pi\Gamma a}{q^2}\frac{(2p+1)!!}{X^p}\, j_p(X) \tag{2}$$

where $j_p(X)$ is the spherical Bessel function of the order $p$ and $X = qr_0$ is a dimensionless parameter depending on the scaling parameter $r_0$. The second term in Eq. (1) is the indirect interaction between the ions which can be considered as a perturbation to the direct Coulomb repulsion and can be expressed in terms of normalized energy-wavenumber characteristic $F_N(q)$

$$u_{\mathrm{SC}}(q) = -\frac{4\pi Z^2 e^2}{q^2} F_N(q) \tag{3}$$

Using the solution of Eq. (2) and combining with Eq. (3), we arrive at the following analytical expression for the static structure factor for 3rd order model i.e. $p = 3$

$$S(q)^{-1} = 1 + \frac{3\Gamma x_0^2}{X^2}\left\{\frac{105}{X^4}\left[\left(\frac{15}{X^2} - 6\right)\frac{\sin X}{X} - \left(\frac{15}{X^2} - 1\right)\cos X\right] - F_N(q)\right\} \tag{4}$$

where $x_0$ is a dimensionless parameter defined by $x_0 = r_0/a$.

The crucial point of our discussion is the non-locality and the choice of core radius of the local model potential. Thus we construct $F_N(q)$ which contains all the information by using a local (Ashcroft) and a non local (Shaw) model potentials separately. In the case of Shaw's non local model, we have used $F_N(q)$ obtained by the same procedure given by Bretonnet and Regnaut[9] while that for Ashcroft's local and energy independent model it is convenient to write $F_N(q)$ explicitly

$$F_N(q) = \left(\frac{q^2 w_0(q)}{4\pi Z e^2}\right)^2\left[1 - \frac{1}{\varepsilon(q)}\right] \tag{5}$$

where the form factor is given by

$$w_0(q) = -\frac{4\pi Ze^2}{q^2}\cos(qR_c)$$

We choose the simplest dielectric function of Hartree so that a clear picture may emerge without any complexity. In Table I, we list our results for structure factors in various choices of ingredients and analyse the numerical results of sodium. The second and third columns of the table I show the divergence for $q = 0$ in the bare OCP system. A similar divergence is observed in $F_N(q)$ exactly compensating it to give a regular behaviour of long-wavelength limit. This reflects the importance of the screening correction in the low-$q$ region.

The height and the position of the first peak can be adjusted with good accuracy by the proper choice of $\Gamma$ and $x_0$. Introducing a local model potential for screening correction creates much trouble in adjusting the height and the position of the first peak. It is important to mention that the choice of core radius $R_c$ in the local model potential is very crucial and sensitive to the height of the first peak as it can be seen from third and fourth columns. The single parameter $R_c$, specifying the electron-ion potential, may be determined by several ways. To compare precisely the role played by both model potentials, $R_c$ has been chosen to fit the first node of Shaw's form factor ($R_c = 1.61$a.u.). In the same way, an empirical cut-off of the screening correction around $2K_{Fj}$ adopted by Chaturvedi *et al.*[4] and Senatore and Tosi[10] was found necessary to restore the first peak to its place. The selection of cut-off position may slightly vary with the choice of core radius, but the empirical cut-off, assumed by these workers, made it possible to achieve the height and the position of the first peak as evident by bracketed values in the fifth column obtained by introducing $F_N = 0.0$ from $q = 2K_F$.

Finally, we introduce the non local model potential of Shaw to obtain the accurate height and position without implying any empirical cut-off, concluding that non-locality plays a dominant role around first peak. A detailed discussion about the selection of parameters applicable to all alkalis will be presented elsewhere. In the last, it is necessary to mention that this comparison is possible due to $x_0^2 = 3.2$, the best possible choice in our opinion, creating a doubt over $x_0^2 = 2.34$ selected by Evans and Sluckin[5]. Our results up to the first peak, particularly in low-$q$ region, are in good agreement with experimental values[11]. However, the amplitude of oscillations in $S(q)$ beyond the first peak are rapidly damped, indicating that this model corresponds to softer repulsive core in the pair potential. As a matter of fact $F_N(q)$ does not influence this range of structure factor as it decay quickly beyond $2K_F$. Further investigations are in progress to find the reason of this failure. Although computer simulations (M.C.) are not well suited to the study of

TABLE I

Comparison of various results for the structure factor of liquid sodium. $F_N(A)$ and $F_N(S)$ correspond to the Ashcroft model potential and Shaw model potential respectively. The parameter $x_0^2 = 3.2$ remains constant for all numerical calculations.

| $q/K_f$ | $F_N = 0.0$ $\Gamma = 187$ | $F_N = 0.0$ $\Gamma = 198$ | $F_N(A)$ $R_c = 1.70$ $\Gamma = 187$ | $F_N(A)$ $R_c = 1.61$ $\Gamma = 187$ | $F_N(A)$ $R_c = 1.61$ $\Gamma = 193.8$ | $F_N(S)$ $\Gamma = 193.8$ | Exp Waseda (1980) | MC Galam & Hansen $\Gamma = 160$ |
|---|---|---|---|---|---|---|---|---|
| 0.1 | $6.6\ 10^{-5}$ | $6.23\ 10^{-5}$ | 0.015 | 0.018 | 0.018 | 0.017 | 0.025 | |
| 0.2 | $2.7\ 10^{-4}$ | $2.54\ 10^{-4}$ | 0.018 | 0.022 | 0.021 | 0.020 | 0.025 | |
| 0.3 | $6.3\ 10^{-4}$ | $5.91\ 10^{-4}$ | 0.019 | 0.023 | 0.022 | 0.021 | 0.026 | |
| 0.4 | 0.001 | 0.001 | 0.020 | 0.024 | 0.023 | 0.023 | 0.027 | |
| 0.5 | 0.002 | 0.002 | 0.022 | 0.026 | 0.025 | 0.025 | 0.028 | ~0.002 |
| 0.6 | 0.003 | 0.003 | 0.024 | 0.029 | 0.028 | 0.027 | 0.031 | |
| 0.8 | 0.007 | 0.006 | 0.030 | 0.036 | 0.035 | 0.035 | 0.037 | ~0.008 |
| 1.0 | 0.013 | 0.012 | 0.040 | 0.049 | 0.048 | 0.047 | 0.047 | |
| 1.2 | 0.026 | 0.025 | 0.058 | 0.071 | 0.069 | 0.069 | 0.060 | ~0.026 |
| 1.4 | 0.054 | 0.051 | 0.091 | 0.111 | 0.108 | 0.111 | 0.094 | ~0.055 |
| 1.5 | 0.080 | 0.076 | 0.118 | 0.144 | 0.139 | 0.147 | 0.122 | ~0.081 |
| 1.6 | 0.120 | 0.114 | 0.158 | 0.190 | 0.185 | 0.199 | 0.165 | ~0.117 |
| 1.8 | 0.297 | 0.286 | 0.320 | 0.366 | 0.358 | 0.405 | 0.312 | ~0.325 |
| 2.0 | 0.830 | 0.822 | 0.841 | 0.843<br>(0.830) | 0.839 | 0.972 | 0.992 | ~1.105 |
| 2.2 | 2.060 | 2.197 | 3.591 | 2.350<br>(2.060) | 2.471 | 2.280 | 2.260 | ~2.720 |
| 2.3 | 2.450 | 2.677 | 9.683 | 3.619<br>(2.450) | 3.999 | 2.705 | 2.707 | ~2.530 |
| 2.4 | 2.310 | 2.508 | 20.323 | 4.340<br>(2.310) | 4.942 | 2.550 | 2.152 | ~1.858 |
| 2.5 | 1.952 | 2.067 | 13.259 | 3.952<br>(1.952) | 4.428 | 1.798 | 1.293 | ~1.350 |
| 3.0 | 1.018 | 1.019 | 1.800 | 1.577<br>(1.018) | 1.608 | 1.040 | 0.635 | ~0.642 |

low-$q$ behaviour they are displayed in last column to compare with bare OCP reference system in Baus and Hansen scheme.

## Acknowledgement

One of us (K.N.K.) acknowledges partial support from French Government for high level scientific fellowship.

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