INFLUENCE OF THE FRIEDEL OSCILLATIONS ON THE STRUCTURE OF LIQUID RUBIDIUM

P. T. Cummings* and P. A. Egelstaff

Department of Physics
University of Guelph
Guelph, Ontario, Canada N1G 2W1

Report #370
July 1981

*Present Address: Department of Mechanical Engineering
State University of New York
Stony Brook, New York 11794
U.S.A.

INFLUENCE OF THE FRIEDEL OSCILLATIONS ON THE STRUCTURE OF LIQUID RUBIDIUM

P. T. Cummings* and P. A. Egelstaff

Department of Physics
University of Guelph
Guelph, Ontario, Canada N1G 2W1

Short Title: Influence of Friedel Oscillations

Physics Abstracts Classification:

C.C.	A6120 A6125	liquid
F.C.	a6120 - ta6125 - w	theory
C.C.	A0520	statistical
F.C.	a0520 - g	mechanics

*Present Address: Department of Mechanical Engineering
State University of New York
Stony Brook, New York 11794
U.S.A.

ABSTRACT

Recent experimental results on liquid rubidium have demonstrated agreement between derivatives of the structure factor with respect to density and momentum transfer as predicted by the Uniform Fluid Model. Using a selection of model fluids (the hard sphere fluid, the Yukawa fluid and a simplified model of liquid metals), each of which is solvable analytically within the mean spherical approximation, we present evidence that the observed experimental behaviour can be explained in terms of the density-dependent Friedel oscillations in the effective inter-ion potential for rubidium.

I. INTRODUCTION

In this paper we are concerned with offering an explanation for the density dependence of the experimental results on the structure of liquid Rb, in terms of Friedel oscillations in the Rb effective pair potential. The experimental results of interest are those of Egelstaff, et al. (1980) in which the structure factor $S(q)$, where q is momentum transfer, was measured on a grid of temperature-density points in the phase plane such that density derivatives of $S(q)$ were obtained. They proceeded to interpret these results in terms of a Uniform Fluid Model (UFM) (introduced by Egelstaff, et al. (1971) to explain less extensive data on rubidium). The UFM can be characterized in the following simple way: for true liquid metal potentials we assume there is a characteristic scaling of r induced by the density dependence of the Fermi wavenumber -- i.e., $k_F \sim \rho^{1/3}$, so it is conceivable that $r \sim \rho^{-1/3}$; hence $g(r)$ the radial distribution function, is a universal function $g(x)$ where $x = r\rho^{1/3}$ and consequently $S(q)$ is a universal function $S(y)$ where $y = q\rho^{-1/3}$. This leads directly to the prediction

$$\rho \frac{\partial S(q)}{\partial \rho} \approx - \frac{q}{3} \frac{\partial S(q)}{\partial q} . \qquad (1)$$

Egelstaff, et al. (1971 and 1980) verified experimentally that liquid Rb did indeed satisfy (1) in the region of the first peak of $S(q)$ [which is the natural domain of validity of (1) if the arguments leading to (1) are correct]. It has also been shown (Egelstaff and

Wang 1972) that the UFM does not agree with data on neon or the Lennard-Jones fluid, probably because the nearest neighbor packing changes with density in these cases.

However, the agreement between the UFM and experiment is not necessarily a definitive test of the assumptions underlying it, since the behaviour (1) may result from factors other than, or in addition to, the density dependence in k_F. In this paper we examine the UFM closely using the model introduced by Cummings (1979) and defined by an effective pair potential between the liquid metal ions, $\phi(x)$, of the form

$$\phi(r) = \begin{cases} \infty & r < \sigma \\ -\dfrac{A\, e^{-z(r-\sigma)}}{r} [\cos 2k_F r + \delta] & r > \sigma \end{cases} \qquad (2)$$

where r is the inter-ion separation, A, z and δ are constants and k_F is the Fermi wavenumber of the electrons given by

$$k_F = 2(3\pi^2 Z\rho)^{1/3} \qquad (3)$$

where Z is the valence and ρ is the number density of the ions. Notice that in (2) it is assumed that the ions have a hard impenetrable core of diameter σ. Whilst (2) is an idealisation of a true liquid metal potential in a number of ways [for a detailed discussion, see Cummings and Stell (1981)], it is nonetheless an attractive model for the examination of the qualitative effect of Friedel oscillations since, as shown by Cummings (1979), the mean spherical approximation

(MSA) can be solved analytically for the potential (2). The MSA is an approximate closure to the Ornstein-Zernike (OZ) equation connecting the total correlation function h(r) and the direct correlation function c(r). The OZ equation is given by

$$h(r) = c(r) + \rho \int d\vec{s}\; c(s)\; h(|\vec{r} - \vec{s}|) \qquad (4)$$

and the MSA for hard core potentials (Lebowitz and Percus 1965) is defined by the two closures

$$g(r) = h(r) + 1 = 0 \qquad r < \sigma \qquad (5)$$

$$c(r) = -\phi(r)/kT \qquad r > \sigma\ . \qquad (6)$$

Equation (5) represents the exact hard core condition; Eq. (6) represents an extrapolation of the asymptotic behaviour of c(r) (Stell 1977) to small separations.

The accuracy and validity of the MSA have been discussed at length elsewhere (Stell 1977). The consensus is that the MSA is unreasonably good in predicting the qualitative structural and thermodynamic behaviour of the fluids to which it is applied. It cannot, however, in general, be relied upon for quantitative accuracy.

We shall present persuasive evidence that the assumptions underlying the UFM are indeed correct within this framework. From the general behaviour of the MSA, there is reason to expect our results will remain true in a qualitative way in an exact treatment of (2). However, the adequacy of the model (2) to reproduce the behaviour of true liquid metals -- in particular, Rb -- must be considered. The

most serious error is the assumption of a hard core: considerable evidence, reviewed by Mountain and Haan (1979), now exists to substantiate the idea that liquid Rb has a relatively soft core compared to noble gases (see also Page, et al. 1969). From the point of view of comparison with experiment, the unfortunate aspect is that the soft-core and Friedel oscillations tend to cancel one another in their effect on a property such as the shape of the first peak in S(q). [For a discussion see Section IV and Cummings and Stell (1981).] The most obvious property in which this cancellation occurs is the magnitude of the peaks in S(q); the Friedel oscillations tending to increase them and the soft core tending to decrease them. Simple perturbation theory (e.g., Barker and Henderson 1967) tends to disregard the role of the attractive part of $\phi(r)$, but this is inappropriate for Fourier components whose wavelength is similar to that of the oscillations in $\phi(r)$. Thus we cannot expect quantitative agreement with experiment for any hard core model. Therefore we test the model by asking whether equation (1) is satisfied.

The effect of the Friedel oscillations can be delineated, however, by comparing the predictions of the model (2) with those of the hard sphere fluid ($A = 0$) and those of the Yukawa fluid ($k_F = 0$, $\delta = 0$) (Cummings and Smith 1979a,b). The latter two fluids can be regarded as simple models of noble gases. Explicitly, the hard sphere potential [$\phi_{HS}(r)$] and the Yukawa potential [$\phi_{YUK}(r)$] are given by

$$\phi_{HS}(r) = \begin{cases} \infty & r < \sigma \\ \\ 0 & r > \sigma \end{cases} \tag{7}$$

$$\phi_{YUK}(r) = \begin{cases} \infty & r < \sigma \\ \\ -\dfrac{B\, e^{-y(r-\sigma)}}{r} & r > \sigma \end{cases} \tag{8}$$

By solving all three models (2), (7) and (8) in the MSA, we are able to observe the explicit effect of the Friedel oscillations; in particular, we are able to see the extent to which (1) is satisfied.

The details of the solution of the MSA for (2) and (8) have been given previously [Cummings 1979 , Cummings and Stell 1981 , Cummings and Smith 1979a,b] and are not repeated here. The MSA for $\phi_{HS}(r)$ is simply the Percus-Yevick approximation (Percus and Yevick 1955) and this has been solved analytically by Wertheim (1963) and Thiele (1963). In Section III we report the results of a series of computations for the potentials $\phi(r)$, $\phi_{HS}(r)$ and $\phi_{YUK}(r)$. Preceding this, in Section II, there is a brief discussion of the salient density dependence of a published potential for Rb (Price, et al. 1970) which provides the focus of the discussion in Section III. The possibility of soft core effects is discussed in Section IV, and our conclusions are summarized in Section V.

II. DENSITY DEPENDENCE OF THE PRICE POTENTIAL

The Price potential for liquid Rb (Price, et al. 1970) has been shown by Mountain (1978) to yield quite accurate structural properties for liquid Rb. On this basis, we assume that the Price potential $\phi_p(r)$ can be considered to be a reasonable representation of the inter-ion effective pair potential. One of the clearly density dependent aspects of this potential is the asymptotic form

$$\phi_p(r) \sim \frac{\cos 2k_F r}{r^3} . \tag{9}$$

We wish to examine a number of other density dependent features of $\phi_p(r)$ which might account for, or contribute to, the observed experimental behaviour (1) for liquid Rb.

A stylized form of the Price potential is shown in Fig. 1. There are four important parameters defined in this figure: the first zero of the potential, σ_1; the second zero of the potential σ_2; the position of the first minimum R_{min}; and the depth of the first minimum ε. If $\phi_p(r)$ takes up the asymptotic form (9) even at short separations, then $\sigma_2 - \sigma_1$ should vary $\sim\rho^{-1/3}$. We are also interested in the behaviour of σ_1, R_{min} and ε as a function of ρ.

The experimental work of Egelstaff, et al. (1980) was concentrated in the density regime $\rho \sim 0.01$ ions Å^{-3}. Hence $\phi_p(r)$ was calculated for a range of density in the vicinity of $\rho = 0.01$. The results are tabulated in Table 1. From this table it is easy to verify the following results:

(i) $\sigma_2 - \sigma_1 \approx \rho^{-1/3}$;

(ii) $\varepsilon \approx \rho^{-1/3}$;

(iii) σ_1 and R_{min} are relatively independent of ρ .

Result (i) implies that the scaling effect of k_F is present even at relatively short separations; result (ii) is clearly an additional scaling property of the Rb potential which must be examined as a possible contributing factor toward (1).

The experimental conditions at which Egelstaff, et al. (1980) found agreement between these derivatives were $0.0098 \leq \rho \leq 0.0108$ Å^{-3} and absolute temperature $328° \leq T \leq 473°$. In Figure 2, the Price potential is shown at a number density $\rho = 0.01036$ Å^{-3}. As noted above, σ_1 for the Price potential is only weakly dependent on ρ. Hence for all the calculations reported here, the potentials $\phi_{HS}(r)$, $\phi_{YUK}(r)$ and $\phi(r)$ were assumed to have a common, fixed hard core diameter of 4.2 Å. Also shown in Figure 2 is the $\phi_{YUK}(r)$ and $\phi(r)$ used in the calculations: $\phi(r)$ was fitted in a least squares fashion to $\phi_p(r)$ over the first minimum; the depth of $\phi_{YUK}(r)$ was assigned to be the same depth as $\phi_p(r)$. In regard to the fitting of $\phi(r)$ to $\phi_p(r)$, it should be pointed out that the functional form (2) is not sufficiently flexible to enable a good fit to $\phi_p(r)$ over a large range. Consequently although the first minimum could be well fitted, there was an over-estimate of the amplitude of the Friedel oscillations over one or two ion diameters. Alternatively, $\phi(r)$ was fitted to $\phi_p(r)$ over the range r = 7 to 10 Å, but this led to a very poor fit of the first minimum

region. Also the latter fitting was found to be unstable: that is, it displayed sensitive behaviour to the number of points included in the fitting procedure. As a consequence of this, fitting in the bowl region only (4.4 Å $\leq$ r $\leq$ 6.4 Å) was used. It is felt that this captures the essential physics of the Price potential: a potential well with density-dependent width and depth, and a potential mound at r $\sim$ 7-8 Å. The main defect seems to be that this mound is too large, and this feature coupled with the hard core seems to generate too tall a peak in S(q) in our calculations. For this reason, and in view of the deficiencies of the potential (2) noted above, we do not make direct comparisons with experimental data, but investigate the conditions under which equation (1) is satisfied.

III. DENSITY DEPENDENCE OF S(q)

In this section we report a series of model calculations on the hard sphere fluid [pair potential $\phi_{HS}(r)$, Eq. (7)], the Yukawa fluid [pair potential $\phi_{YUK}(r)$, Eq. (8)] and the model liquid metal [pair potential $\phi(r)$, Eq. (1)]. The derivatives

$$\rho \frac{\partial S(q)}{\partial \rho} \quad \text{and} \quad -\frac{q}{3}\frac{\partial S(q)}{\partial q} \tag{10}$$

will be evaluated and compared for each model. The calculations covered a large range of possible origins for the observed behaviour (1).

3.1 Total Density Dependence in $\phi(r)$

In this calculation, the Price potential $\phi_p(r)$ was calculated at densities $\rho - \Delta\rho$, ρ, $\rho + \Delta\rho$ (where $\rho = 0.01036$ Å^{-3} and $\Delta\rho = 0.0002$ Å^{-3}). The parameters for the model liquid metal potentials were determined at these three densities by fitting in the bowl region, and the MSA was solved for T = 423° using the techniques previously described (Cummings 1979, Cummings and Stell 1981), thus yielding three structure factors $S(q;\rho - \Delta\rho)$, $S(q;\rho)$, $S(q;\rho + \Delta\rho)$. The derivatives in (10) were then obtained from the formulae

$$\rho \frac{\partial S(q)}{\partial \rho} \cong \rho \left[\frac{S(q;\rho + \Delta\rho) - S(q;\rho - \Delta\rho)}{2\Delta\rho}\right] \tag{11}$$

$$-\frac{q}{3}\frac{\partial S(q)}{\partial q} \cong -\frac{q}{3}\left[\frac{S(q + \Delta q;\rho) - S(q - \Delta q;\rho)}{2\Delta q}\right] \tag{12}$$

Because the potentials $\phi(r)$ were obtained by fitting $\phi_p(r)$ at three neighbouring densities, each $\phi(r)$ carries full density dependence: i.e., in k_F, A, z and δ. The results are shown in Figure 3, with the same derivatives for $\phi_{HS}(r)$ shown for comparison. There are two noteworthy features:

(i) for hard spheres, there is clearly no agreement between (11) and (12) while for the model liquid metal there is near perfect agreement.

(ii) the magnitudes of the derivatives for the model liquid metal are much higher (by a factor of about 2) than the hard sphere derivatives which agree with the magnitude of the experimental data (Egelstaff, et al., 1971).

This latter point was anticipated in the discussion in Sections I and II where it was pointed out that tha model potential (2) is artificial in having a hard core and a large mound at 8 Å: (ii) is one of the consequences of this artificiality. Nevertheless the difference in the agreement between the derivatives (11) and (12) for the hard sphere and model liquid metal systems (both solved in the MSA) is attributable only to the difference in the potentials -- that is, to the inclusion of the Friedel oscillations.

There are, at this point, a number of questions which can be asked: what are the precise factors in $\phi(r)$ which determine the agreement between (11) and (12)? Is it simply that $k_F \sim \rho^{1/3}$, or does it depend on the potential being oscillatory? That is, if one considered a Yukawa fluid (8) with $y \sim \rho^{1/3}$, would agreement be obtained between the derivatives (11) and (12)? How important is the fact that the well depth $\varepsilon \sim \rho^{-1/3}$? We answer these questions in the calculations reported below.

We focus on the density dependence in various parameters in $\phi_{YUK}(r)$ and $\phi(r)$. The Price potential $\phi_P(r)$ was calculated at $\rho = 0.01036$ Å^{-3}, and the liquid metal potential (2) was fitted as before, yielding A, z and δ, [k_F being determined by (3)]. The Yukawa parameter B was set to be the well depth of $\phi_P(r)$ at this density and y was set equal to z, the decay in $\phi(r)$. In all the ensuing calculations, z and δ [in $\phi(r)$] were considered fixed at their values for $\rho = 0.01036$. The density-dependence of the remaining

parameters [A and k_F in $\phi(r)$, B and y in $\phi_{YUK}(r)$] was studied by separate calculations covering the following classes:

CLASS I: A, B, k_F, y all density independent

CLASS II: A, B $\sim \rho^{-1/3}$; with k_F, y density independent

CLASS III: A, B density independent; k_F, $y \sim \rho^{1/3}$

CLASS IV: A, B $\sim \rho^{-1/3}$; k_F, $y \sim \rho^{1/3}$

In this way, tentative answers can be given to the questions raised in the preceding paragraph: the MSA is used in all cases with T = 423°K.

3.2 Class I

We shall ask two questions: first is the observed agreement in Figure 3 simply the result of $\phi(r)$ having an attractive bowl? If so, the Yukawa fluid should show agreement between (11) and (12). On the scale of Figure 4 the Yukawa results are indistinguishable (except near k = 0) from those of hard spheres (Fig. 3), for which there was no agreement between (11) and (12). Secondly, how much of the agreement between (11) and (12) is caused by the fact that $\phi(r)$ is oscillatory? The results for ϕ_{YUK} are shown by the dashed and dot-dash lines in Figure 4, and do not agree. However for $\phi(r)$ there is good agreement between (11) and (12) in Figure 4 which may be the result of the pair potential having an oscillatory tail. This fact is discussed in Section V.

3.3 Class II

This class of calculations examines the effect of the density dependence in well depth, as noted in Section II for $\phi_p(r)$. The results are shown in Figure 5. Both the Yukawa and the model liquid metal results are virtually unchanged from Figure 4. We conclude, therefore, that, by itself, the density dependence in the well depth has no appreciable effect on the agreement between (11) and (12).

3.4 Class III

In the brief introduction to the UFM given in Section I, the key point was the distance scaling of the potential with $\rho^{-1/3}$ as a result of $k_F \sim \rho^{1/3}$. If this were the only fact resulting in the agreement (1), then this argument would hold for a Yukawa potential (9) with $y \sim \rho^{1/3}$. As shown by the results in Figure 6, this is not the case -- if $y \sim \rho^{1/3}$ for the Yukawa fluid we obtain derivatives (11) and (12) which are virtually unchanged from Figures 4 and 5. For the model liquid metal, however, it can be seen that allowing $k_F \sim \rho^{1/3}$ yields an improvement over the agreement in Figures 4 and 5. Thus the agreement reported in Section 3.1 depends mainly upon the oscillatory form of the potential, and full agreement requires $k_F \sim \rho^{1/3}$ as well. In the real case the relative importance of the $k_F \sim \rho^{1/3}$ factor may be greater since the importance of the oscillatory factor in this model calculation is probably overestimated due to the large amplitude of the mound at r = 8 Å.

3.5 Class IV

From Sections 3.3 and 3.4 we conclude that the density dependence of the well depth is unimportant both for $\phi_{YUK}(r)$ and $\phi(r)$, and that the density dependence of y is unimportant in $\phi_{YUK}(r)$; by contrast, the density dependence of k_F in $\phi(r)$ was found to be, comparatively, quite important. The calculations of this section were designed to check whether in combination these density dependences are more significant than when acting independently. As seen by comparing Figs. 6 and 7, the answer is no, both for $\phi_{YUK}(r)$ and $\phi(r)$.

IV. EFFECTS DUE TO THE SOFT CORE

A factor which might contribute to the agreement (1) is the soft core of the rubidium potential as discussed in Section I. One possible way of introducing soft core effects would be through perturbation theory (e.g., Barker and Henderson 1967), but to first order the change in S(q) from, e.g., hard spheres, is insufficient to yield agreement with (1). Nevertheless this treatment is significant in showing that the magnitudes of S(q) and its derivatives are moved closer to the experimental values by including a soft core. In another attempt we investigated the soft sphere model of Hoshino (1980), but we found that the calculated derivatives were unphysical and concluded that this model was not applicable to our problem.

In a third attempt we used the "soft core Yukawa potential" in

the MSA where:

$$\phi_{SCY}(r) = \begin{cases} \infty & r < \sigma \\ + \dfrac{B\, e^{-y(r-\sigma)}}{r} & r > \sigma \end{cases} \qquad (13)$$

We found that if the parameters were chosen so that $\phi_{SCY}(r)$ had roughly the same shape as $\phi_P(r)$ for r less than the first minimum (R_{min}) in $\phi_P(r)$, it was not possible to fit either S(q) or its derivatives. However if the parameters were chosen arbitrarily (e.g., $B = 7.23\ kT\sigma$; $y\sigma = 8.9$; $\sigma = 4.2$ Å) it was possible to obtain a reasonable fit to the experimental data on both S(q) and its derivatives. But in this case $\phi_{SCY}(r)$ was unlike $\phi_P(r)$, being much steeper for $r < R_{min}$. In addition for some values of r we observed $\phi_{SCY}(r) >> kT$ making the corrections to MSA quite important (e.g., Stell 1977). Consequently we concluded that this agreement was artificial, and that the potential (13) did not lead to the agreement (1) if consistency was demanded.

It would be desirable to treat these effects in a more positive way, but it may be that extensive computer simulations are required to do this.

V. DISCUSSION

The above calculations lead to the following conclusion: the features of a liquid metal potential which lead to the experimentally observed agreement (1) are the existence of Friedel oscillations (see

Section 3.2) and their density dependence via k_F (see Section 3.4). As noted in Cummings and Stell (1981) the effect of Friedel oscillations appears to be to order the fluid to a greater extent than in their absence. Our physical picture thus assumes that the primary effect of the Friedel oscillations is to localize the positions of nearest neighbours to a greater extent than occurs for a non-oscillatory potential. For example the existence of the potential mound beyond σ_2 in Figure 1, will lead to a greater localization of nearest neighbours in the range $\sigma_1 < r < \sigma_2$ than would be the case for a noble gas. As increases, $\sigma_2 - \sigma_1 \sim \rho^{-1/3}$ and so the localization of nearest neighbours will scale similarly with density. In essence, this is the behaviour reflected in the experimental observation (1). Since all the density-dependence in $\phi(r)$ [and $\phi_p(r)$] arises from the contribution of the electrons, it can be seen that the electrons play a greater role in determining liquid metal structure than is emphasised by the hard sphere model, for example. The fact that the UFM has been found to be applicable only to simple liquid metals is an illustration of this property.

All our conclusions have been based on results for model systems solved in the MSA: thus our conclusion can only be regarded as accurate to the extent that the MSA is reliable for making model comparisons and that the liquid metal model represents liquid rubidium fairly. Ultimately, however, they should be verified conclusively by computer simulation.

ACKNOWLEDGEMENTS

PTC acknowledges the financial support of the Commonwealth Scientific and Industrial Research Organization (CSIRO) Australia through a CSIRO Post-Doctoral Fellowship. This work was supported by a research grant from the Natural Sciences and Engineering Research Council of Canada, and by the National Science Foundation and the Donors of the Petroleum Research Fund, administered by the American Chemical Society. The authors take pleasure in acknowledging helpful discussions with Professor George Stell, and the collaboration of Drs. J-B Sück and J. B. Hayter in the calculations for the soft core Yukawa potential.

REFERENCES

Barker J A and Henderson D 1967 J. Chem. Phys. 47 4714.

Cummings P T 1979 J. Phys. F: Metal Physics 9 1477.

Cummings P T and Smith E R 1979a Molec. Phys. 38 997.

Cummings P T and Smith E R 1979b Chem. Phys. 42 241.

Cummings P T and Stell G 1981 Molec. Phys., in press.

Egelstaff P A Page D I and Heard C R T 1971 J. Phys. C: Solid St. Phys. 4 1453.

Egelstaff P A Sück J-B Gläser W McPherson R and Teistma A 1980 Proceedings of LAM4 J. Physique 41 C8-222.

Egelstaff P A and Wang S S 1972 Can. J. Phys. 50 2461.

Hoshino K 1980 J. Phys. C: Solid St. Phys. 13 3097.

Lebowitz J L and Percus J K 1966 Phys. Rev. 144 251.

Mountain R D and Haan S W 1979 J. Res. Nat. Bur. Stand. 84 439.

Mountain R D 1978 J. Phys. F: Metal Physics 8 1637..

Page D I Egelstaff P A Enderby J E and Wingfield B R 1969 Phys. Letts. 29A 296.

Percus J K and Yevick G J 1958 Phys. Rev. 110 1.

Price D L Singwi K S and Tosi M P 1970 Phys. Rev. B2 2983.

Stell G 1977 Chapter 2 of Modern Theoretical Chemistry Vol. 5A: Statistical Mechanics ed. B Berne (New York: Plenum).

Thiele E 1963 J. Chem. Phys. 39 474.

Wertheim M S 1963 Phys. Rev. Letts. 10 321.

TABLE I

Variation of the parameters σ_1, σ_2, R_{min} and ε with density for the Price potential for Rb

ρ Å^{-3}	σ_1 Å	σ_2 Å	R_{min} Å	ε/k °K
0.0100	4.412	7.246	5.175	-405
0.0102	4.412	7.229	5.175	-402
0.0104	4.412	7.215	5.175	-400
0.0106	4.411	7.194	5.150	-397
0.0108	4.411	7.178	5.150	-394
0.0110	4.410	7.161	5.150	-392
0.0112	4.410	7.142	5.150	-390

FIGURE CAPTIONS

Figure 1. A typical liquid metal potential showing the parameters σ_1, σ_2, R_{min} and ε (for discussion, see Section II).

Figure 2. The potential $\phi_p(r)$ for liquid Rb at $\rho = 0.01036$ Å^{-3} (— — — — —) compared with three model potentials; the model liquid metal potential $\phi(r)$ (— • — • —) [Eq. (2)], the Yukawa potential $\phi_{YUK}(r)$ (— — — —) [Eq. (8)] and the hard sphere potential $\phi_{HS}(r)$ (————) [Eq. (7)]. All model potentials have an impenetrable core of diameter $\sigma = 4.2$ Å.

Figure 3. Derivatives of the structure factor for $\phi(r)$ and $\phi_{HS}(r)$: $-\frac{q}{3}\frac{\partial S(q)}{\partial q}$ for $\phi(r)$ (————) and $\phi_{HS}(r)$ (— • — • —), $\rho\frac{\partial S(q)}{\partial \rho}$ for $\phi(r)$ (— x — x —) and $\phi_{HS}(r)$ (— — — —).

Figure 4. Derivatives of the structure factor for $\phi(r)$ and $\phi_{YUK}(r)$ for Class I (see Section 3.2): $-\frac{q}{3}\frac{\partial S(q)}{\partial q}$ for $\phi(r)$ (————) and $\phi_{YUK}(r)$ (— — —); $\rho\frac{\partial S(q)}{\partial \rho}$ for $\phi(r)$ (— x — x —) and $\phi_{YUK}(r)$ (— — — —).

Figure 5. As for Figure 4, with Class II (see Section 3.3).

Figure 6. As for Figure 4, with Class III (see Section 3.4).

Figure 7. As for Figure 4, with Class IV (see Section 3.5).

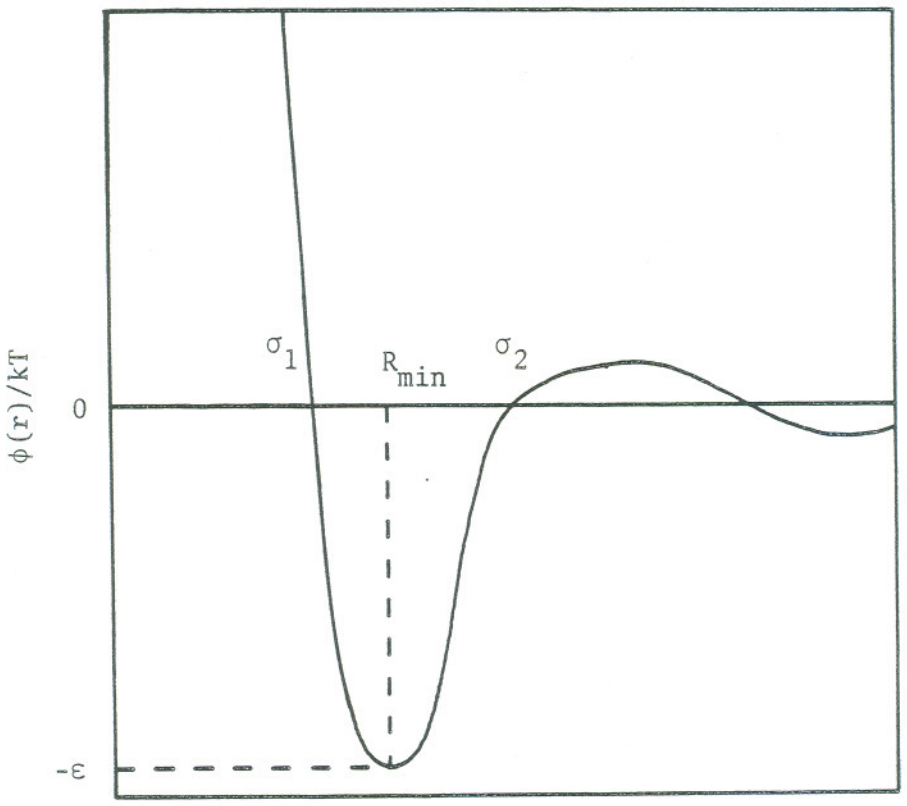

Figure 1

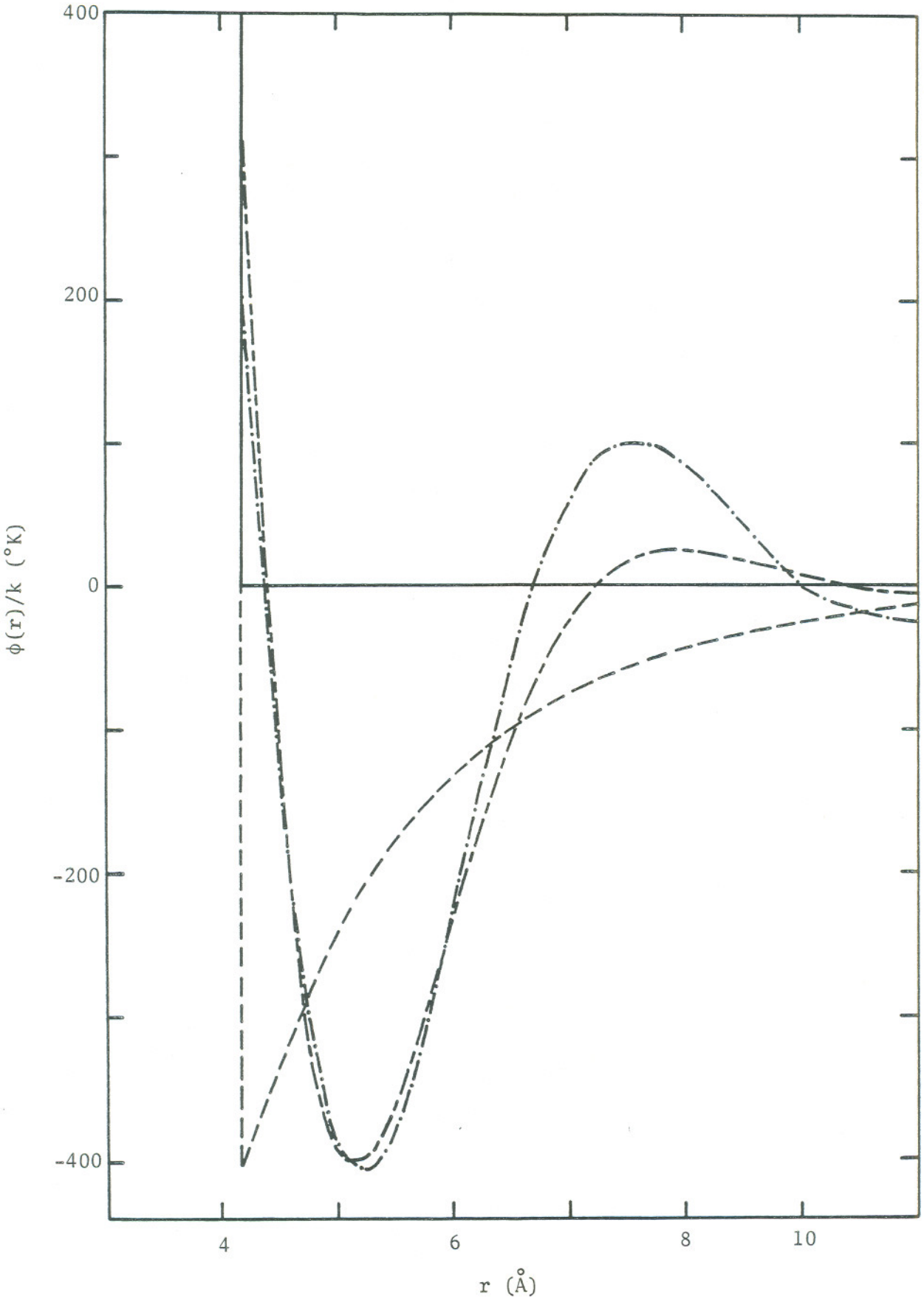

Figure 2

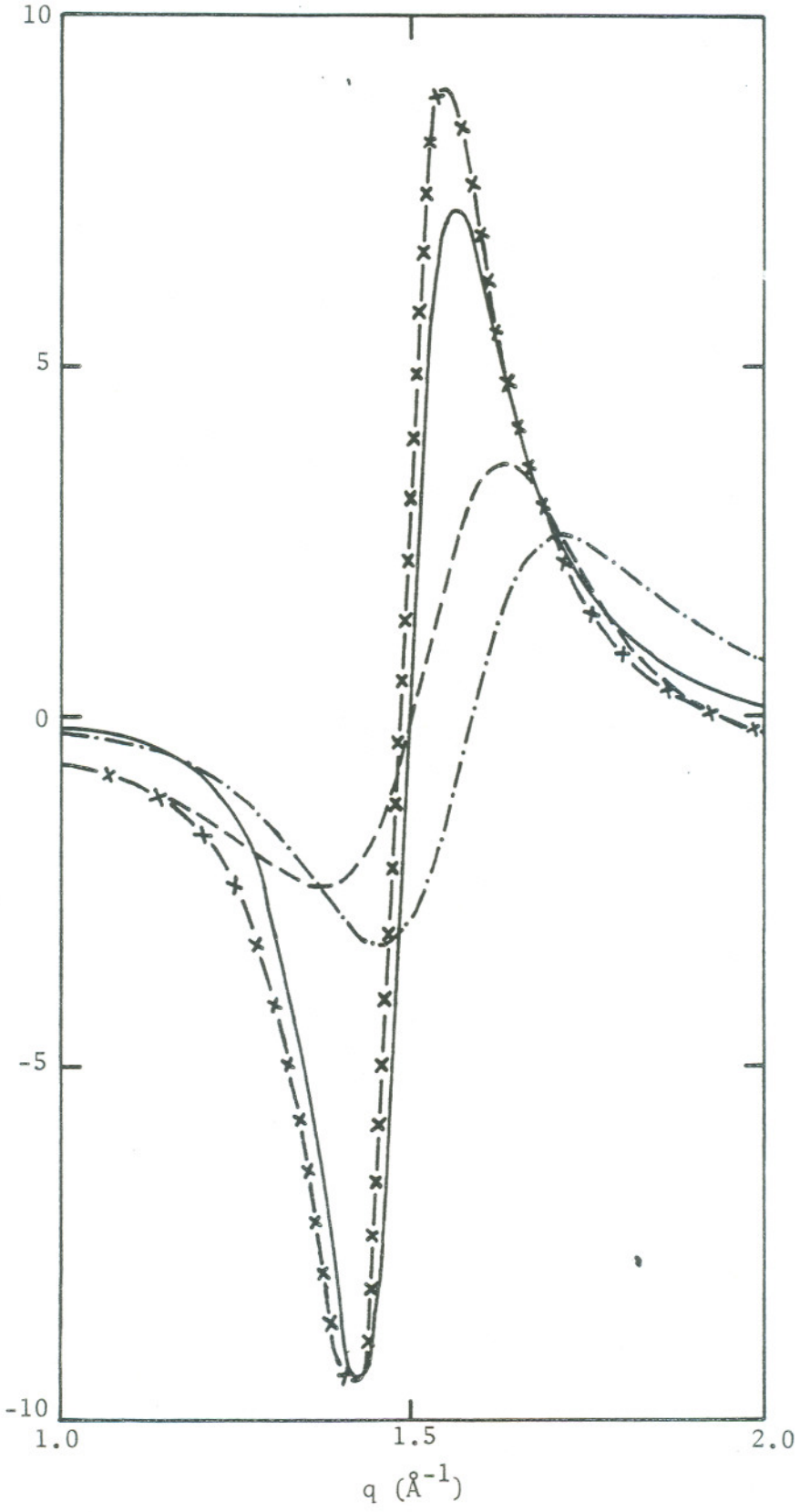

Figure 3

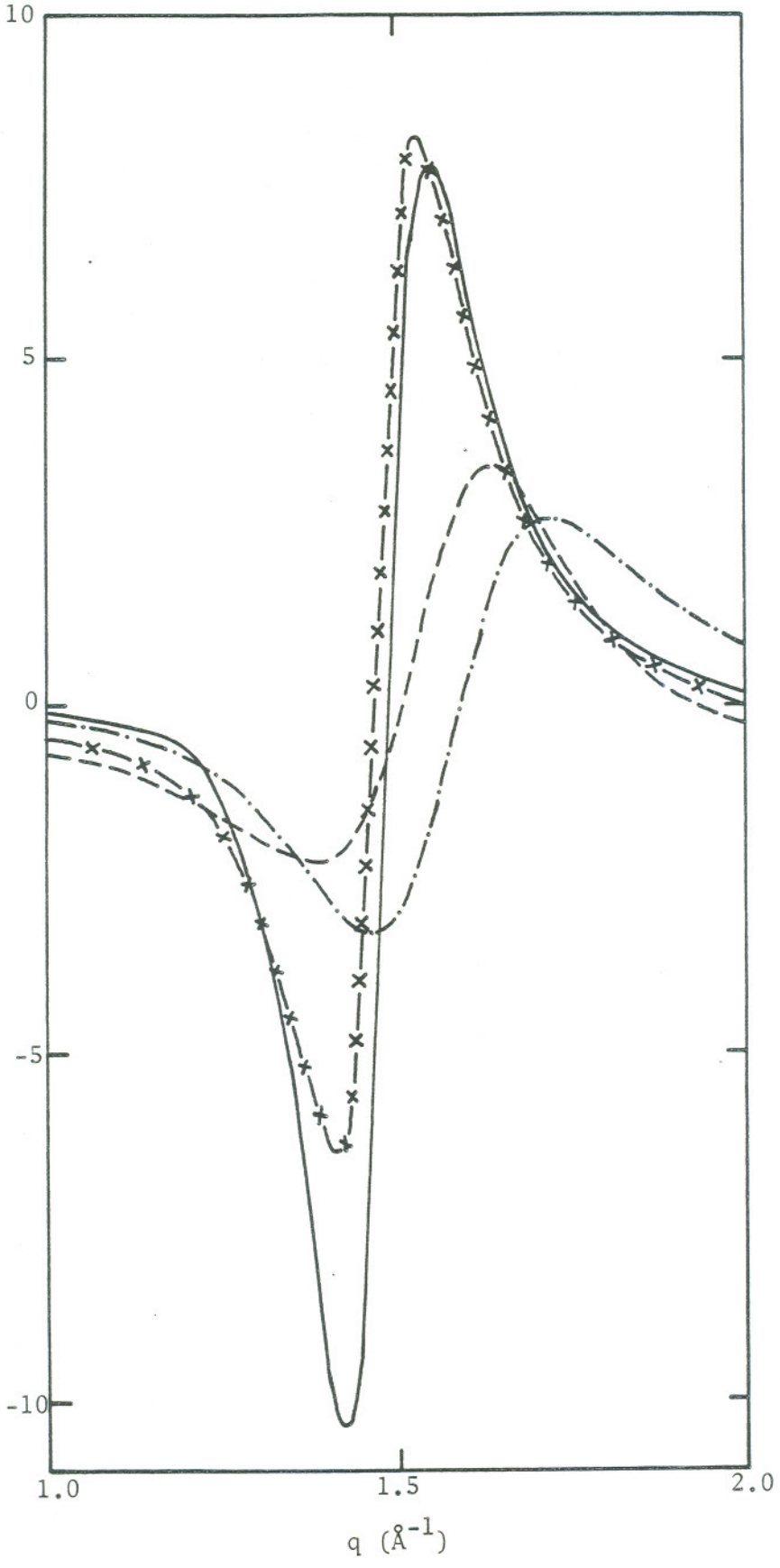

Figure 4

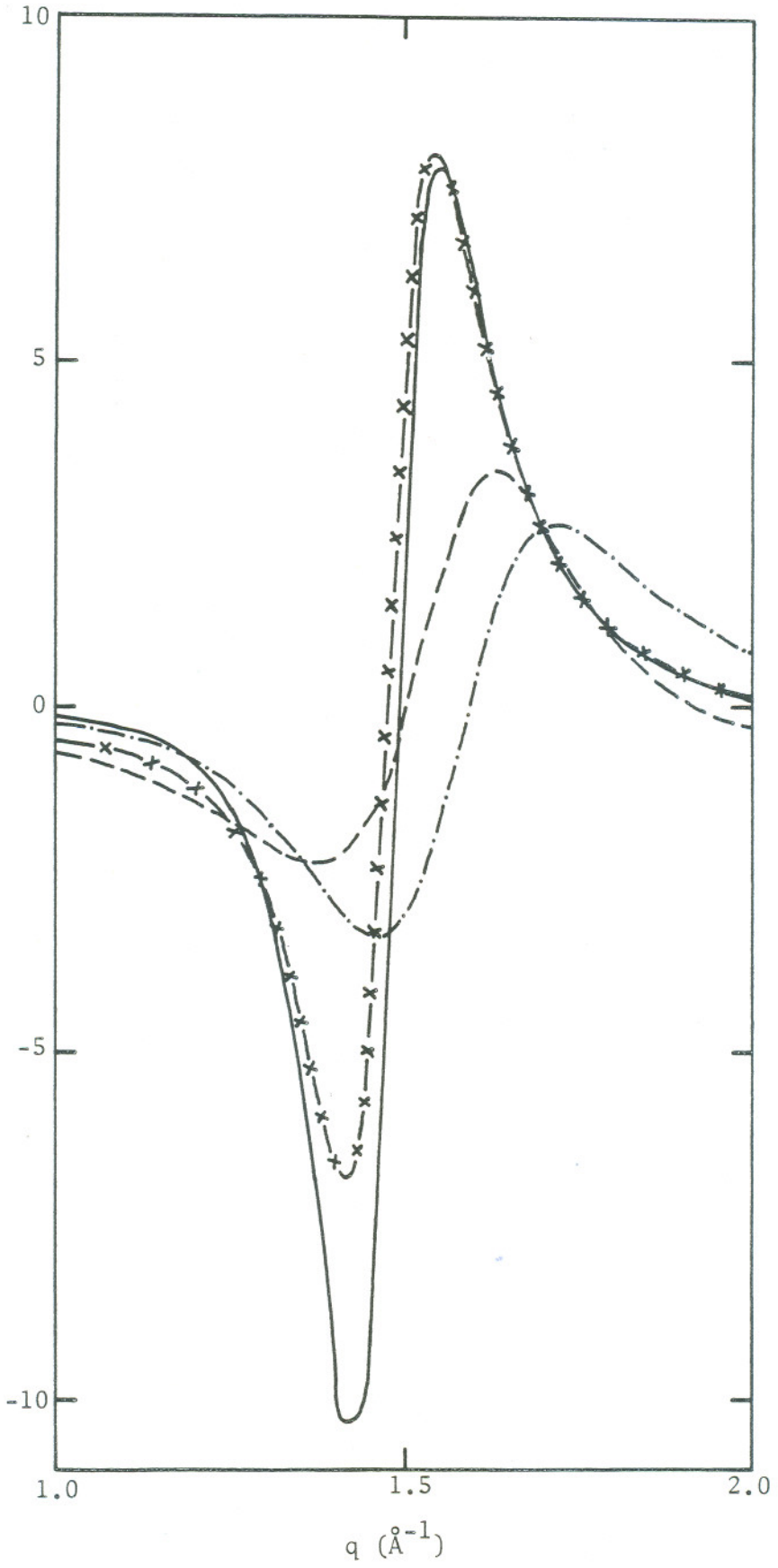

Figure 5

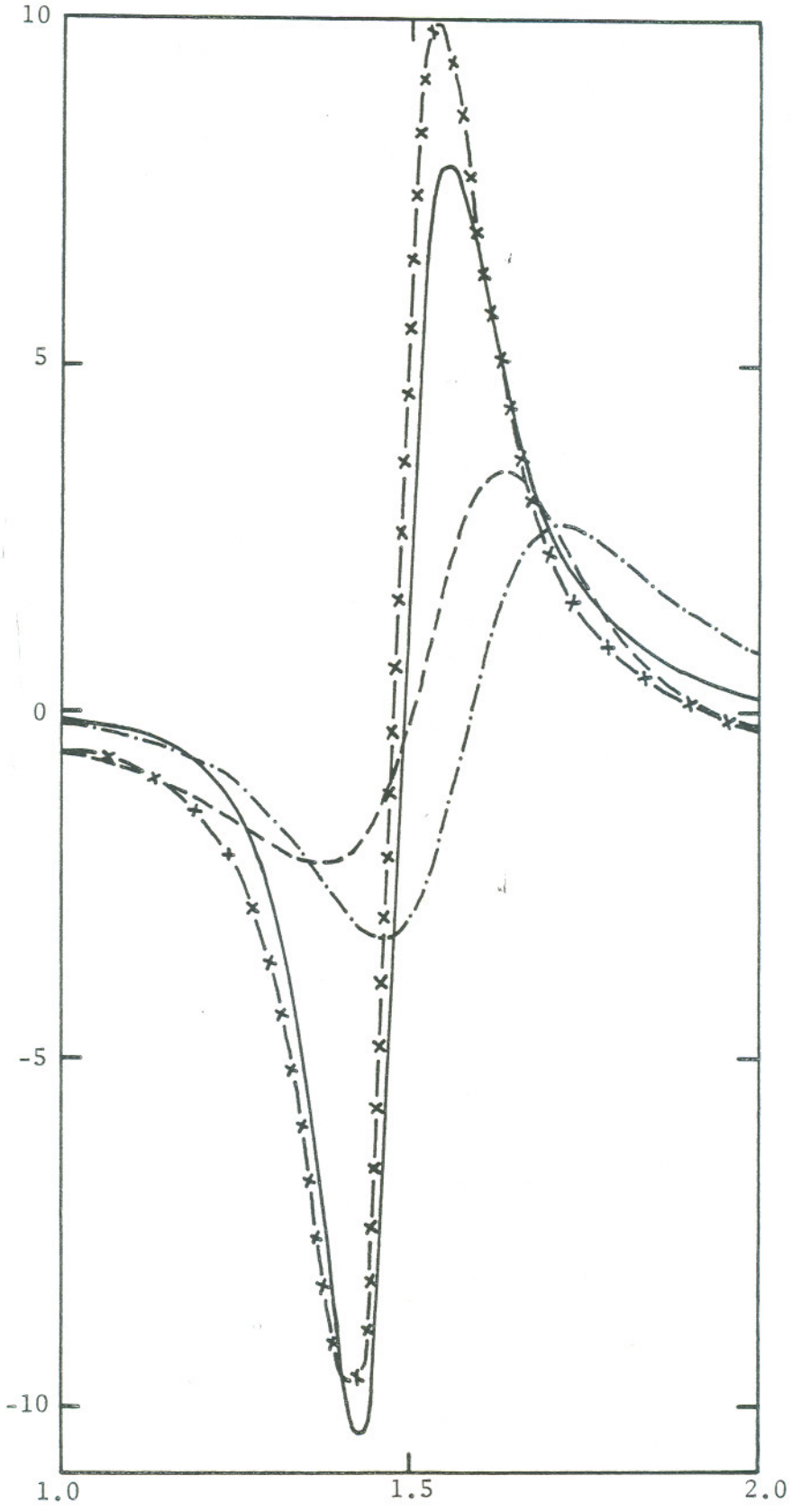

Figure 6

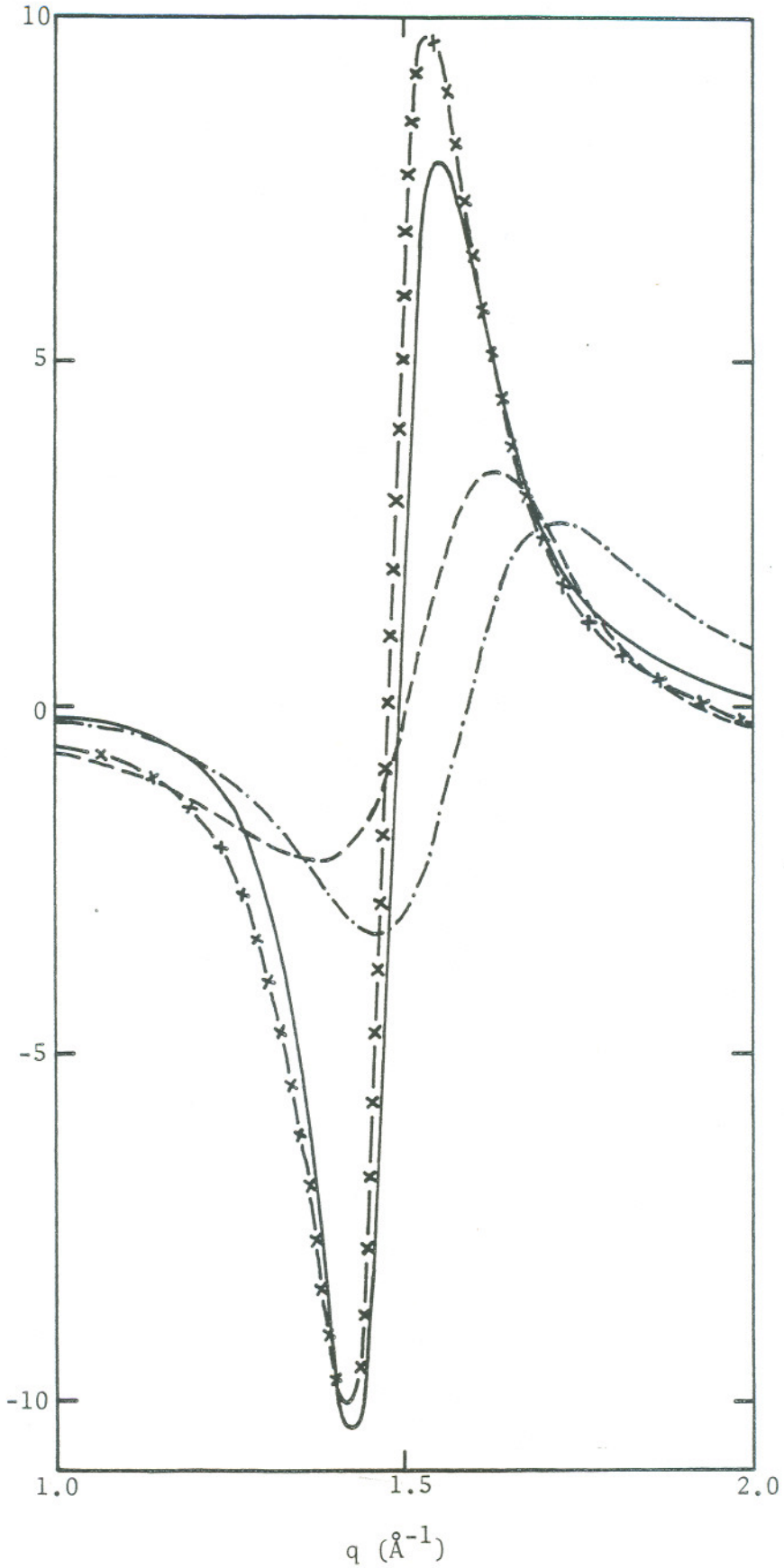

Figure 7