

Gibbs-Bogoliubov variational scheme calculations for the liquid structure of 3d transition metals

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1992 J. Phys.: Condens. Matter 4 5359

(<http://iopscience.iop.org/0953-8984/4/24/005>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.96

The article was downloaded on 11/05/2010 at 00:17

Please note that [terms and conditions apply](#).

Gibbs–Bogoliubov variational scheme calculations for the liquid structure of 3d transition metals

J L Bretonnet†, G M Bhuiyan and M Silbert

School of Physics, University of East Anglia, Norwich NR4 7TJ, UK

Received 6 December 1991, in final form 20 February 1992

Abstract. The results of calculations of the static structure factor $S(q)$ for liquid 3d transition metals are presented. These have been studied using effective inter-ionic pair potentials, proposed by two of the authors (JLB and MS), that combine the empty-core model used to describe the nearly-free-electron band and a d-band contribution deduced via an inverse scattering approach. They have potential wells that are shallower and shifted towards the larger values of r than the corresponding Wills–Harrison potentials used by other authors. The fluid aspects are modelled through a charged hard-sphere reference system optimized via the Gibbs–Bogoliubov variational scheme.

The results for $S(q)$ agree reasonably well with the available experimental data. The optimized values found for the hard-sphere diameters reveal that the ions never sample the hard cores, confirming earlier findings on the need to use a soft-core reference system for liquid transition metals.

1. Introduction

In earlier studies we have applied the Gibbs–Bogoliubov (GB) variational scheme with a hard-sphere (HS) fluid chosen as the reference system to the three series of liquid transition metals (Aryasetiawan *et al* 1986, Bretonnet and Derouiche 1991 (BD)). In the first paper the effective Hamiltonian for the ions is based on a semiempirical tight-binding model originally proposed by Ducastelle (1970). The effective Hamiltonian in the second paper is based on a first-principles study by Wills and Harrison (1983) (WH), which uses separate treatments for the s–p and the d states leading to an effective pair potential that also takes into account the effect of s–d hybridization.

A similar study to that of BD was carried out by Hausleitner and Hafner (1988) using a modified WH potential with a hard-sphere Yukawa (HSY) reference fluid. These authors have shown that the HSY fluid yields a better variational upper bound to the Helmholtz free energy than the HS reference fluid, suggesting that a soft-core reference system is more appropriate for liquid transition metals.

Regnaut (1989) has also used the WH potential to carry out an analysis of the structure of the 3d liquid transition metals by means of the so-called WCA–ORPA perturbation theory (see Andersen *et al* 1976). He finds that the predictions of the WH potential depend critically on the cancellation between the two large repulsive and attractive contributions. Specifically, Regnaut finds that the purely repulsive WCA

† On study leave from the Laboratoire de Physique des Liquides Métalliques, Université de Metz, 57045 Metz Cédex 1, France.

scheme leads to results that are similar to those obtained with the HSY reference fluid. However, incorporating the attractive, mainly d-band, contribution via ORPA fails to produce results for the early 3d elements as the structure factor diverges in the long-wavelength limit.

Regnaut's findings were confirmed by the recent work of Hausleitner *et al* (1991), who have shown that modern thermodynamically self-consistent integral equation theories of liquids also lead to similar difficulties to those of the WCA-ORPA in describing the structure of transition metals with half-filled and less than half-filled d bands. Moreover, their molecular dynamics simulations using a modified WH potential fail to produce reasonable results for liquid Ti and V. It appears that the root of the problem is the very deep potential well predicted by the WH potential for its first minimum and its position. Hausleitner *et al* (1991) concluded that improvements in the description of the structure of liquid transition metals require a shallower potential well shifted towards a larger value of r than that predicted by WH.

The preceding results have encouraged us to develop a new simple effective interaction for transition metals which possesses the correct attributes for a good description of the liquid structure (Bretonnet and Silbert 1991) and through which we intend to carry out a systematic study of the properties of liquid transition metals.

In this paper we report the results of the GB variational scheme with a charged hard-sphere (CHS) reference system. This system is essentially the same as the one-component plasma (OCP) model except that it includes the size effect of the positive ions interacting via a Coulomb potential in a uniform background of negative charge. The OCP has been used by Khanna and Cyrot-Lackmann (1979) and Chaturvedi *et al* (1981a, b, c) to describe the structure of liquid transition metals as well as by Itami and Shimoji (1984) and by Itoh *et al* (1986) to study their thermodynamic properties. In our work we appeal to the analytic solution obtained by Palmer and Weeks (1973) for the CHS system in the mean spherical approximation.

In the next section we describe the GB variational scheme as used in this work. In section 3 we present the results of our calculation for the 3d transition series and we show that the use of our potential yields reasonably good agreement with the experimental structure. Finally, we complete the paper with a brief discussion of our results.

2. The Gibbs-Bogoliubov variational scheme

Assuming that the effective Hamiltonian H for the ions may be written as the sum of the Hamiltonian of the reference system H^{CHS} , which in our case is a CHS system, plus the rest of the effective Hamiltonian then the GB inequality states that the Helmholtz free energy F of the system is given by

$$F \leq F^{\text{CHS}} + \langle H - H^{\text{CHS}} \rangle_{\text{CHS}} \quad (2.1)$$

where F^{CHS} denotes the free energy of the reference system and the brackets a canonical ensemble average over the reference system.

Equation (2.1) may be simplified by considering only the structure-dependent part of the free energy, F_s , which may now be written as

$$F_s \leq F_s^{\text{CHS}}(\eta) + E_M(\eta) + E_{bs}(\eta) \quad (2.2)$$

where E_M and E_{bs} are the Madelung and band structure energies, respectively, calculated by using the CHS structure factor. The packing fraction η is chosen as the variational parameter.

F_s^{CHS} is obtained by integrating the excess internal energy $U^{CHS}(\eta)$ as given in Palmer and Weeks (1973), namely

$$U^{CHS}(\eta)/k_B T = -(1/24\eta)\{(1 + \eta - \frac{1}{5}\eta^2)K^2 + (1 + 2\eta)K[1 - (1 + [2(1 - \eta)^3 K/(1 + 2\eta)^2])^{1/2}]\}. \quad (2.3)$$

At a given temperature T and number density ρ , $\eta = \pi\rho\sigma^3/6$ where σ is the hard-sphere diameter. In addition, for this system, the Debye-Hückel inverse length K is given by

$$K = (24\eta\beta Z_s^2 e^2/\sigma)^{1/2} \quad (2.4)$$

where $\beta = (k_B T)^{-1}$ and $Z_s e$ is the ionic charge. F_s^{CHS} is given by

$$\begin{aligned} \frac{F_s^{CHS}}{k_B T} = & \frac{\eta(4 - 3\eta)}{(1 - \eta)^2} - \frac{K^2}{24\eta}(1 + \eta - \frac{1}{5}\eta^2) \\ & - \frac{(1 + 2\eta)^3}{36\eta(1 - \eta)^3} \left[1 - \left(1 + \frac{2(1 - \eta)^3}{(1 + 2\eta)^2} K \right)^{3/2} \right] - \frac{(1 + 2\eta)}{12\eta} K \end{aligned} \quad (2.5)$$

when the Carnahan-Starling (1969) equation is used for the neutral hard-sphere system.

In equation (2.2) we adopt the procedure in appendix 1 to calculate $E_M(\eta)$, so that

$$E_M(\eta) = \frac{Z_s^2 e^2}{\pi} \int [S^{CHS}(q; \eta)^{-1}] dq - U^{CHS}(\eta). \quad (2.6)$$

The structure factor $S^{CHS}(q; \eta)$ may be written in terms of the Fourier transform of the Ornstein-Zernike direct correlation function

$$S^{CHS}(q; \eta) = 1/[1 - \rho\tilde{c}^{CHS}(q; \eta)] \quad (2.7)$$

where $\rho\tilde{c}^{CHS}(q; \eta)$, in the mean spherical approximation, may be written in closed form (for the argument Q) as

$$\rho\tilde{c}^{CHS}(Q; \eta) = \frac{24\eta}{Q^6} \sum_{i=1}^6 A_i J_i(Q). \quad (2.8)$$

Explicit expressions for the coefficients A_i and the functions $J_i(Q)$ of the dimensionless variable $Q = q\sigma$ are given in appendix 2. We note that equations (2.5) and (2.8) reduce to the corresponding HS expressions on taking the limit $K = 0$.

The band structure energy $E_{bs}(\eta)$ is written as

$$E_{bs}(\eta) = -\frac{Z_s^2 e^2}{\pi} \int dq S^{CHS}(q; \eta) F_N(q) \quad (2.9)$$

where $F_N(q)$ is the normalized energy-wavenumber characteristic

$$F_N(q) = (q^2/4\pi\rho Z_s e^2)^2 \omega_0^2(q) (1 - 1/\epsilon(q)) [1 - G(q)]^{-1}. \quad (2.10)$$

In equation (2.10) $\omega_0(q)$ denotes the form factor, which is derived from our model potential. As with the WH potential, we use separate treatments for the s-p and the d states. The former are treated within the empty-core model potential. The latter are obtained by using an inverse scattering approach (Bretonnet and Silbert 1991). Actually there are several methods available for deducing potentials from the knowledge of the elastic scattering phaseshifts (see Marchenko 1963). We have used the distorted plane-wave method developed by Swan (1967) (see also Oli 1988) in which the potential inside the core radius R_c is expanded as a finite Dirichlet series of short-range functions. A good estimate of the potential is obtained by retaining only the first two terms of the series. In addition, we require the potential and its first derivative to be continuous at $r = R_c$. The resulting form factor is

$$\begin{aligned} \omega_0(q) = 4\pi\rho a^3 \{ & B_1 H_1(q)/(1 + a^2 q^2)^2 + 8B_2 H_2(q)/(1 + 4a^2 q^2)^2 \} \\ & - (4\pi\rho Z_s e^2/q^2) \cos(qR_c) \end{aligned} \quad (2.11)$$

where

$$\begin{aligned} B_1 &= (Z_s e^2/R_c)(1 - 2a/R_c) \exp(R_c/a) \\ B_2 &= (2Z_s e^2/R_c)(a/R_c - 1) \exp(R_c/2a) \end{aligned}$$

and

$$\begin{aligned} H_n(q) = 2 - \exp(-R_c/na) \{ & ((R_c/na)(1 + n^2 a^2 q^2) + (1 - n^2 a^2 q^2)) \\ & \times \sin(qR_c)/naq + (2 + (R_c/na)(1 + n^2 a^2 q^2)) \cos(qR_c) \} \end{aligned}$$

where the parameter a is a measure of the softness of the repulsive potential.

The dielectric screening function $\epsilon(q)$ is given by

$$\epsilon(q) = 1 - (4\pi e^2/q^2) \chi(q) [1 - G(q)] \quad (2.12)$$

where $\chi(q)$ is the Lindhard function and $G(q)$ is the local-field correction taken from Ichimaru and Utsumi (1981).

We now turn to the choice of parametrization and the presentation of the results.

3. Results

In order to carry out the minimization procedure the parameters Z_s , R_c and a must be specified. For the number of free electrons we take the non-integer value $Z_s = 1.2$ for all the elements in the 3d series. This falls within the range of values that are acceptable according to Moriarty (1990). A non-integer $Z_s > 1$ value is assumed to include the effect of s-d hybridization (Itami and Shimoji 1984).

The form factor given by equation (2.11) and its related effective pair potential are fairly insensitive to changes in the core radius R_c . A compilation of the ratio

R_c/r_0 , for a large number of liquid metals, shows that it spans the narrow range 0.47–0.52. Therefore we assume that $R_c = r_0/2$ for all the elements in this study, where r_0 ($r_0^3 = 3/4\pi\rho$) is the Wigner-Seitz radius. This choice of R_c is also consistent with the approximate relationship given by Hafner and Heine (1983),

$$D \sim 2R_c + 2\lambda_{\text{TF}} \quad (3.1)$$

where D is the repulsive core diameter and λ_{TF} is the Thomas-Fermi screening radius.

For the remaining parameter a we adopt the following procedure. We adjust the low- q region of the structure factor calculated within the random-phase approximation (RPA) to the experimental data. The RPA structure factor is given by

$$S^{\text{RPA}}(q) = \{1 - \rho[\tilde{c}^{\text{CHS}}(q) - \beta\tilde{u}_{\text{sc}}(q)]\}^{-1} \quad (3.2)$$

where

$$\tilde{u}_{\text{sc}}(q) = -(4\pi Z_s^2 e^2 / q^2) F_N(q)$$

is the electronically screened interaction between the ions.

In the long-wavelength limit we have the following closed form for the RPA structure factor

$$[S^{\text{RPA}}(0)]^{-1} = 1 - 24\eta(A_1/3 + A_2/4 + A_3/5 + A_4/6 + A_5/8) + A_6/2 + 4\pi\beta\rho Z_s^2 e^2 (R_c^2 - 2P + \pi h^2/4me^2 K_F - \gamma_0/K_F^2) \quad (3.3)$$

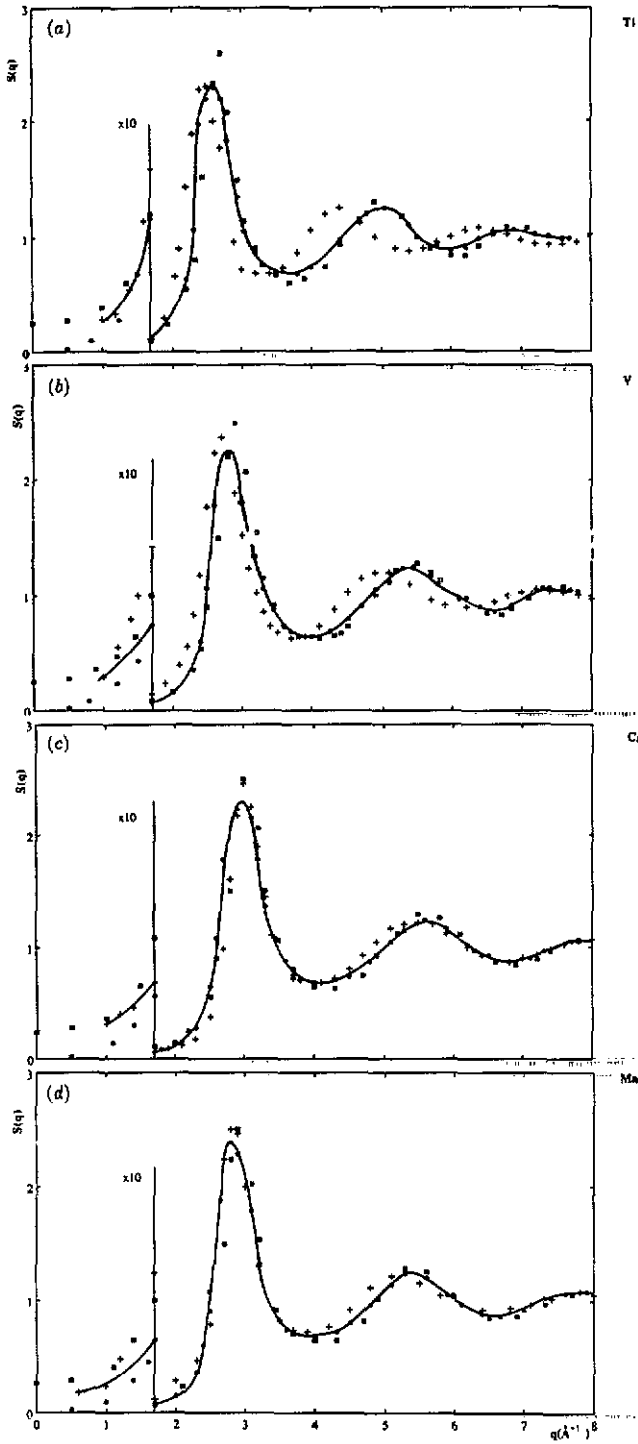
where

$$P = (a^3/Z_s e^2) [B_1 H_1(0) + 8B_2 H_2(0)]$$

and γ_0 is a dimensionless parameter obtained from the local-field correction $G(q)$ (see equation (4) in Ichimaru and Utsumi (1981)).

Table 1. Input data for the variational calculations of the liquid 3d transition metals (columns 2 to 5): temperature, T ; number density, ρ ; core radius, R_c ; and the adjusted potential softness parameter, a (see text). Output results for the optimized packing fractions η (columns 6 and 8) and free energies $F/k_B T$ (columns 7 and 9) using the CHS and HS reference systems.

	T (K)	$10^{-3}\rho$ (au)	R_c (au)	a (au)	η^{CHS}	$(F_s/k_B T)^{\text{CHS}}$	η^{HS}	$(F_s/k_B T)^{\text{HS}}$	η^{S}
Sc	1812	6.94	1.626	0.301	0.418	-251.456	0.452	-249.984	
Ti	1943	7.67	1.573	0.287	0.420	-268.667	0.455	-267.059	0.406
V	2175	9.75	1.452	0.267	0.415	-228.487	0.445	-227.138	0.436
Cr	2130	10.82	1.402	0.259	0.410	-229.061	0.445	-227.678	0.445
Mn	1517	9.80	1.449	0.276	0.418	-243.144	0.445	-241.680	0.449
Fe	1809	11.22	1.386	0.264	0.410	-182.534	0.435	-181.602	0.398
Co	1768	11.69	1.367	0.260	0.412	-213.854	0.440	-212.612	0.408
Ni	1726	11.84	1.361	0.262	0.410	-205.658	0.438	-204.508	0.396



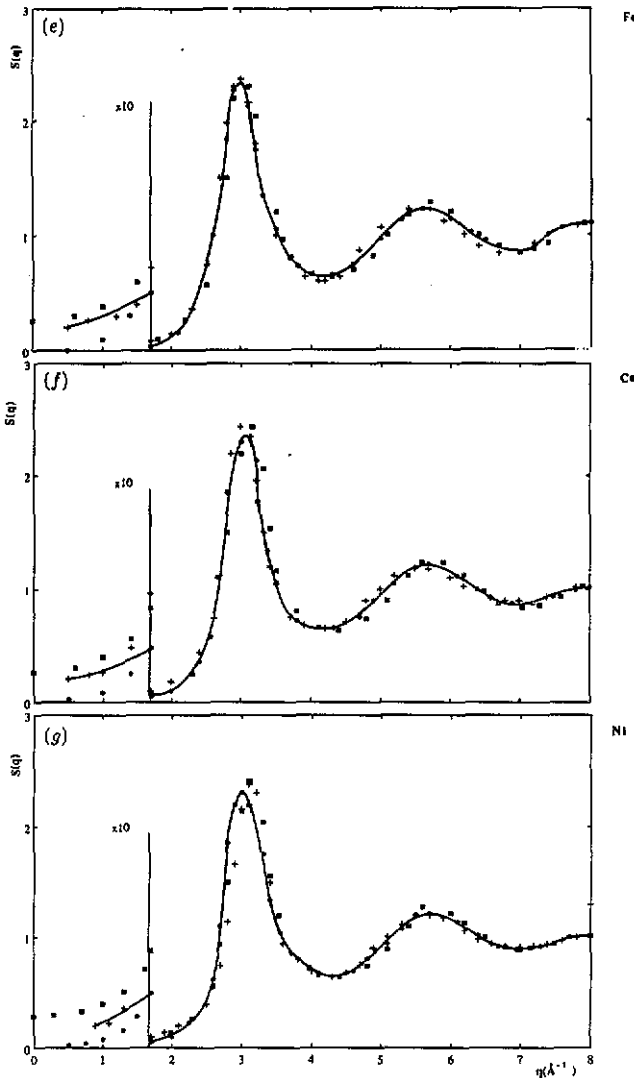


Figure 1. Static structure factors $S(q)$ for the liquid 3d transition metals: full curves, CHS results; squares, HS results; crosses, experiment, Waseda (1981). The following elements were investigated; (a), Ti; (b), V; (c), Cr; (d), Mn; (e), Fe; (f), Co; (g), Ni.

We now proceed with the variational scheme, as follows. The minimization procedure is repeated for different values of the parameter a until $S^{\text{RPA}}(q)$ reproduces the experimental data in the low- q regime. The values of the optimized packing fractions η^{CHS} and the excess free energies $(F_s/k_B T)^{\text{CHS}}$ thus obtained are presented in table 1, which also contains the relevant input data. We have also included in table 1 the values of the optimized packing fractions η^{HS} and the excess energies $(F_s/k_B T)^{\text{HS}}$ obtained when using an HS reference system.

We note that, in all cases, $\eta^{\text{CHS}} < \eta^{\text{HS}}$. This, as we shall see below, results in first peak heights of $S(q)$ which, for our CHS reference system, are about 5% lower than those found experimentally. Similar trends were observed by Hausleitner and Hafner

(1988) when comparing their HSY reference system with the HS results, although they used a different model potential.

The structure-dependent free energy obtained by using the CHS reference system yields a lower variational upper bound than the HS reference fluid. Nonetheless, the differences between F_s^{CHS} and F_s^{HS} are small and of the same magnitude as found by Hausleitner and Hafner (1988) for the 3d liquid transition metals, and by Li *et al* (1986) for both the alkali and the polyvalent liquid simple metals, when the results of using the HSY and HS reference fluids are compared.

We now turn to the structure factors for the 3d liquid transition metals, which are shown in figures 1(a) to (g). Our $S^{\text{CHS}}(q)$ are compared with the x-ray experimental data of Waseda (1981) and the HS results. According to experiment the height of the principal peak for the other systems in the 3d row does not change significantly from one element to another; the damping of the oscillations is less pronounced than in the alkalis thus reflecting a slightly harder repulsive potential. At a more detailed level a shift in the position of the principal peak towards smaller q in Ti and V, *vis-à-vis* the other elements, cannot be explained simply by their large atomic volumes. However, Waseda (1981) states that the quality of the experimental data for the early elements in the 3d series is not as good as for the remainder of the series.

The CHS calculations shift the position of the principal peak of $S(q)$ towards smaller values of q —as compared with HS results—bringing the calculated results nearer to the experimental data for the elements in the middle of the 3d row. In contrast, no improvement with regard to the HS results is observed for both the early 3d elements and for Ni. For the former the shift of $S(q)$ towards smaller q is not enough while for Ni it is too much.

Meyer *et al* (1984) and more recently Hausleitner and Hafner (1988) found that the best HSY fit to the experimental data is obtained when the value of the potential at the hard-core diameter, $u(r = \sigma)$, is several times the thermal energy $k_B T$; namely, when the hard core of the reference potential is never sampled. This suggests that the reference parameters reflect the relevant properties of the effective pair interaction. We find a similar trend when using the CHS reference system. The value of $u(r = \sigma)$ for our potential lies in the range 7–10 $k_B T$ as is shown for the typical elements Ti, Mn and Ni (respectively early, middle and late elements in the 3d row) in figure 2. In our case $u(\sigma)/k_B T = 9, 7.7$ and 7 for Ti, Mn and Ni, respectively.

Finally, we note that whereas the values of σ and a differ from one element to another in the 3d series, the ratios a/r_0 and σ/r_0 are nearly constant at 0.095 and 1.52, respectively. This could indicate the existence of a universal scaling feature for the structure factors of liquid transition metals. We are currently checking whether similar trends are observed in the other transition-metal series.

4. Discussion

During the past five or six years there have been a few systematic studies of the structure and thermodynamic properties of liquid transition metals. It is as if, all of a sudden, there is a realization amongst liquid metals theorists that the study of these systems has become a soluble problem.

The published papers are attempts to probe either methods of liquid state theory and/or potentials borrowed from solid state studies—i.e., to probe approaches that have proved successful in the past. Slowly, from piecing together the modest findings

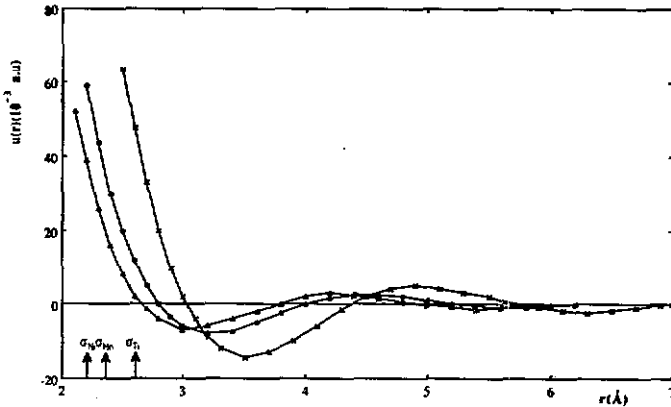


Figure 2. Effective inter-ionic pair potentials for liquids Ti (crosses), Mn (circles) and Ni (triangles). The arrows indicate the positions of the hard cores for each system.

from each of these studies, a few important patterns are emerging as to what is needed to construct a good theory of liquid transition metals. This work only adds another page to this evolving story.

The most important lesson emerging from these studies is that potentials that have been successful in solid state studies are not easily transferable to the liquid state. There are, roughly speaking, two classes of theories. Those like the WH, obtained from pseudopotential theory, and those deduced by Moriarty (1988, 1990) from density functional theory (generalized pseudopotential theory), yield potential wells which are too deep and whose minima are at relatively small values of r to cause major problems when used in conjunction with integral equation theories of liquids (see Hausleitner *et al* 1991). The many-body potentials of Finnis and Sinclair (1984) and Daw and Baskes (1984) produce the correct type of attractive pairwise contributions, but there are difficulties when it comes to incorporating the repulsive contribution in a self-consistent manner, and also in trying to construct an effective pair interaction which takes care, albeit approximately, of the many-body contributions to the cohesive energy. Actually, it is remarkable that these two different approaches, leading to such different potentials, are equally successful in describing the same systems in the solid state.

Whereas there is strong evidence that the contributions of multi-ion terms are necessary in the study of solid transition metals (Pettifor 1989), we believe that—at the very least as a practical proposition—progress in the understanding of their liquid state properties may only come by using effective pair potentials that take approximate account of the important many-body contributions. The simple effective pair potential used in this work belongs to this category. Its first minimum is shallower, and at larger values of r , than the corresponding WH potential.

The use of this potential, together with a CHS reference system, within the GB variational approach has shown that it yields the correct trends for the liquid structure. We are currently investigating the liquid structure by using the same potential and with an integral equation theory of liquids; preliminary results for the early 3d liquid transition metals are promising and will be reported on completion.

Acknowledgments

This work was supported by the EEC under their Science Plan (grant No SC1000341). One of us (GMB) thanks the Commonwealth Scholarship Commission for the provision of a research studentship.

Appendix 1. Structure-dependent excess free energy

With the CHS reference system, the GB inequality is

$$F \leq F^{\text{CHS}}(\eta) + U(\rho) + \frac{1}{2}\rho \int d^3r g^{\text{CHS}}(r; \eta)[u(r) - u^{\text{CHS}}(r; \eta)]. \quad (\text{A1})$$

On adding and subtracting one to the integrand of equation (A1), and defining

$$U^{\text{CHS}}(\eta) = \frac{1}{2}\rho \int d^3r g^{\text{CHS}}(r; \eta)u^{\text{CHS}}(r; \eta)$$

and

$$\tilde{u}(q) = \int d^3r u(r)e^{iq \cdot r}$$

equation (A1) becomes

$$F \leq F^{\text{CHS}}(\eta) + U(\rho) + \frac{1}{2}\rho \int d^3r [g^{\text{CHS}}(r; \eta) - 1]u(r) + \frac{1}{2}\rho \tilde{u}(q=0) - U^{\text{CHS}}(\eta). \quad (\text{A2})$$

Using Parseval's theorem and the definition of the structure factor

$$S(q) = 1 + \rho \int d^3r [g(r) - 1]e^{iq \cdot r}$$

the third term on the right-hand side of (A2) is

$$\frac{1}{2} \frac{1}{(2\pi)^3} \int d^3q [S^{\text{CHS}}(q; \eta) - 1]\tilde{u}(q). \quad (\text{A3})$$

Since

$$\tilde{u}(q) = (4\pi Z^2 e^2/q^2)[1 - F_N(q)]$$

and defining

$$E_{\text{bs}}(\eta) = -\frac{1}{16\pi^3} \int d^3q (4\pi Z^2 e^2/q^2) S^{\text{CHS}}(q; \eta) F_N(q) \quad (\text{A4})$$

and

$$E_{\text{M}}(\eta) = \frac{1}{16\pi^3} \int d^3q [S^{\text{CHS}}(q; \eta) - 1] (4\pi Z^2 e^2/q^2) - U^{\text{CHS}}(\eta) \quad (\text{A5})$$

the structure-dependent excess free energy F_S is given by

$$F_S \leq F_S^{\text{CHS}}(\eta) + E_{\text{bs}}(\eta) + E_{\text{M}}(\eta)$$

while the remaining term is a volume-dependent contribution.

Appendix 2. Coefficients of the CHS analytic solution for the Fourier transform of the direct correlation function, $c^{\text{CHS}}(q)$

We quote below, for completeness, the expressions for the coefficients of the CHS Palmer and Weeks (1973) analytic solution of $c^{\text{CHS}}(q)$ given in equation (2.8):

$$A_1 = -(1 + 2\eta)^2 / (1 - \eta)^4 + R^2 / 4(1 - \eta)^2 - (1 + \eta)RK / 12\eta - (5 + \eta^2)K^2 / 60\eta$$

$$A_2 = 6\eta M^2 \quad A_3 = \frac{1}{6} K^2 \quad A_4 = \frac{1}{2} \eta (A + K^2 U)$$

$$A_5 = \frac{1}{60} \eta K^2 \quad A_6 = -K^2$$

with

$$R = [(1 + 2\eta)/(1 - \eta)] \left[1 - (1 + 2(1 - \eta)^3 K / (1 + 2\eta)^2)^{1/2} \right]$$

$$M = R^2 / 24\eta - (1 + \eta/2) / (1 - \eta)^2$$

$$U = -(1/12\eta) (1 + \eta - \eta^2/5) - (R/12\eta K)(1 - \eta).$$

The quantities $J_i(Q)$, which are functions of the dimensionless variable $Q = q\sigma$, are

$$J_1(Q) = Q^3(\sin Q - Q \cos Q)$$

$$J_2(Q) = Q^2[2Q \sin Q - (Q^2 - 2) \cos Q - 2]$$

$$J_3(Q) = Q[(3Q^2 - 6) \sin Q - (Q^2 - 6)Q \cos Q]$$

$$J_4(Q) = [(4Q^2 - 24)Q \sin Q - (Q^4 - 12Q^2 + 24) \cos Q + 24]$$

$$J_5(Q) = (1/Q^2)[6(Q^4 - 20Q^2 + 120)Q \sin Q \\ - (Q^6 - 30Q^4 + 360Q^2 - 720) \cos Q - 720]$$

$$J_6(Q) = (\cos Q) / Q^2.$$

References

- Andersen H C, Chandler D and Weeks J D 1976 *Adv. Chem. Phys.* **35** 105
 Aryasetiawan F, Silbert M and Stott M J 1986 *J. Phys. F: Met. Phys.* **16** 1419
 Bretonnet J L and Derouiche A 1991 *Phys. Rev. B* **43** 8924
 Bretonnet J L and Silbert M 1991 *Phys. Chem. Liq.* at press
 Carnahan N F and Starling K E 1969 *J. Chem. Phys.* **51** 635
 Chaturvedi D K, Rovere M, Senatore G and Tosi M P 1981a *Physica B* **111** 11
 Chaturvedi D K, Senatore G and Tosi M P 1981b *Let. Nuovo Cimento* **30** 47
 — 1981c *Nuovo Cimento B* **62** 375
 Daw and Baskes 1984 *Phys. Rev. B* **29** 6443
 Ducastelle F 1970 *J. Physique* **31** 1055
 Finnis M W and Sinclair J E 1984 *Phil. Mag.* **A 50** 45
 Hafner J and Heine V 1983 *J. Phys. F: Met. Phys.* **13** 2479
 Hausleitner C and Hafner J 1988 *J. Phys. F: Met. Phys.* **18** 1025
 Hausleitner C, Kahl G and Hafner J 1991 *J. Phys.: Condens. Matter* **3** 1589
 Ichimaru S and Utsumi K 1981 *Phys. Rev. B* **24** 7385
 Itami T and Shimoji M 1984 *J. Phys. F: Met. Phys.* **14** L15

- Itoh H, Yokoyama I and Waseda Y 1986 *J. Phys. F: Met. Phys.* **16** L113
Khanna S N and Cyrot-Lackmann F 1979 *J. Physique* **40** L45
Li D H, Moore R A and Wang S F 1986 *Phys. Lett.* **118A** 405
Marchenko V A 1963 *The Inverse Scattering Theory* (New York: Academic)
Meyer A, Silbert M and Young W H 1984 *Phys. Chem. Liq.* **13** 293
Moriarty J A 1988 *Phys. Rev. B* **38** 3199
— 1990 *Phys. Rev. B* **42** 1609
Oli B A 1988 *Nuovo Cimento D* **10** 891
Palmer R G and Weeks J D 1973 *J. Chem. Phys.* **58** 4171
Pettifor D G 1989 *Phys. Rev. Lett.* **63** 2480
Regnaut C 1989 *Z. Phys. B* **76** 179
Swan P 1967 *Nucl. Phys. A* **90** 436
Waseda Y 1981 *The Structure of Non-crystalline Materials* (New York: McGraw-Hill)
Wills J M and Harrison W A 1983 *Phys. Rev. B* **28** 4363