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# Bridge Function in Modified Hypernetted Chain Approximation Related to Structure Factor in Liquid Metals

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An approximate expression is given for the bridge function in the modified hypernetted chain approximation in terms of the structure factor  $S(k)$  in liquid metals. Asymptotically, it is argued that in liquid metals such as Rb with a well defined collective mode the bridge function falls off as  $r^{-4}$  at large distances.

Some time ago, de Angelis and March<sup>1</sup> proposed a simple, though plainly approximate, procedure whereby the pair potential  $\phi(r)$  can be extracted from structure data for liquid metals. This so-called inverse problem, stemming from the work of Johnson and March,<sup>2,3</sup> has recently been re-opened by making use of the modified hypernetted chain theory.<sup>4,5</sup> In this theory, one writes

$$h - c = \frac{\phi - U}{k_B T} + B \quad (1)$$

where  $h = g(r) - 1$  is the total correlation function,  $c(r)$  is the Ornstein-Zernike direct correlation function while  $U(r)$  is the potential of mean force, related to the pair function  $g(r)$  by the Boltzmann factor

$$g(r) = \exp(-U(r)/k_B T). \quad (2)$$

The remaining term in Eq. (1) is the so-called bridge function, which has been discussed particularly by Rosenfeld and Ashcroft.<sup>6</sup>

The purpose of this work is to point out that the bridge term  $B(r)$ , which has been discussed recently by Bernasconi *et al.*<sup>7</sup> in the context of relating the vacancy formation energy in hot close-packed metallic crystals to the liquid structure factor  $S(k)$  at melting, can be approximated, when the treatment of de Angelis and March is valid, directly in terms of  $S(k)$ .

The procedure is to employ Eq. (6) of the work of de Angelis and March,<sup>1</sup> namely

$$\phi(r) = U(r) + \frac{k_B T}{8\pi^3 \rho} \int [S(k) - 1]^2 \exp(\mathbf{i}k \cdot \mathbf{r}) \, d\mathbf{k} \quad (3)$$

in Eq. (1). Then, taking Fourier transforms we can write for the bridge term  $\tilde{B}(k)$  in  $k$  space the result

$$\tilde{B}(k) = -\tilde{c}(k)[S(k) - 1]^2. \quad (4)$$

One consequence of this simple approximate formula (4) is that if we adopt the small  $k$  expansion proposed by Matthai and March<sup>8</sup> for liquid metals with a well defined collective mode, namely

$$S(k) = S(0) + s_1 k + s_2 k^2 + \dots \quad (5)$$

then it follows from Eq. (5) inserted into Eq. (4) that

$$\tilde{B}(k) = \tilde{B}(0) + \text{constant } k + O(k^2) \quad (6)$$

and hence, by Fourier transform, the bridge term  $B(r)$  falls off at large  $r$  as  $r^{-4}$ . In the light of this long-range behaviour, care is clearly needed in extracting  $\phi(r)$  for metals by using the modified hypernetted chain theory for liquid metals such as Rb with a well established collective mode, as is also clear from the work of Senatore and March.<sup>9</sup>

Since it may appear to the reader that the above argument rests crucially on the admittedly quite approximate result (3) of Ref. 1, it is of interest to point to the work of Ballone *et al.*<sup>10</sup> on molten salts, and referred to by Bernasconi *et al.*<sup>7</sup> for metals, namely that asymptotically for a Coulomb liquid at large  $r$ :

$$B(r) \sim \text{constant} \iint h(r')h(r'')h(|\mathbf{r} - \mathbf{r}'|)h(\mathbf{r} - \mathbf{r}'')h(|\mathbf{r}' - \mathbf{r}''|) \, d\mathbf{r}' \, d\mathbf{r}'' \quad (7)$$

Inserting the Fourier transform of  $h(r)$  into Eq. (7), i.e. essentially  $[S(k) - 1]$ , though the argument differs in important details from that based on Eq. (3), the use of the small  $k$  expansion in Eq. (5) again leads to a decay of  $B(r)$  at large  $r$  as  $r^{-4}$ .

In summary, the inverse problem for liquid metals, which was discussed quite recently in Refs 4 and 5, will have to incorporate the fact that the bridge term is itself a function of  $S(k)$ , and in particular in liquid metals with a

collective mode it will have a long-range tail. Nevertheless, the problem of extracting the pair potential remains, of course, of major interest in such metals.

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