

where $\beta = 1/k_B T$, with k_B Boltzmann's constant. This equation must be supplemented with an approximation for $b(r, \sigma_1, \sigma_2)$, the so-called bridge function, whose formal definition as an infinite series in density¹⁵ offers only modest practical guidance. Most approximate closures for c define b implicitly.

The numerical evaluation of the OZ equation is simpler in Fourier transform representation, which deconvolutes the \mathbf{r} integral. Thus, in transform space, Eq. (3) becomes

$$\begin{aligned} \tilde{\gamma}(k, \sigma_1, \sigma_2) &= \rho \int_0^\infty d\sigma_3 f(\sigma_3) [\tilde{c}(k, \sigma_1, \sigma_3) \\ &\quad + \tilde{\gamma}(k, \sigma_1, \sigma_3)] \tilde{c}(k, \sigma_3, \sigma_2), \end{aligned} \quad (5)$$

with one remaining integration. We note that the Fourier transform of a circularly symmetric function in two dimensions becomes a Hankel transform,

$$\tilde{w}(k) = 2\pi \int_0^\infty dr r w(r) J_0(kr), \quad (6)$$

where $J_0(x)$ is the zeroth-order Bessel function; the inverse of (6) is

$$w(r) = \frac{1}{2\pi} \int_0^\infty dk k \tilde{w}(k) J_0(kr). \quad (7)$$

The final integration in Eq. (5) can also be eliminated and the evaluation of the OZ equation reduced to algebra by now expanding all σ -dependent functions in orthogonal polynomials $p_j(\sigma)$, $j=0,1,2,\dots$, defined such that

$$\int_0^\infty d\sigma f(\sigma) p_i(\sigma) p_j(\sigma) = \delta_{ij}, \quad (8)$$

where δ_{ij} is the Kronecker delta. Then with

$$\tilde{\gamma}(k, \sigma_1, \sigma_2) = \sum_{i,j=0}^{\infty} \tilde{\gamma}_{ij}(k) p_i(\sigma_1) p_j(\sigma_2) \quad (9)$$

and a similar expansion of $\tilde{c}(k, \sigma_1, \sigma_2)$, Eq. (5) becomes

$$\tilde{\gamma}_{ij}(k) = \rho \sum_l [\tilde{c}_{il}(k) + \tilde{\gamma}_{il}(k)] \tilde{c}_{lj}(k), \quad (10)$$

or, in matrix notation,

$$\tilde{\Gamma}(k) = \rho [\tilde{C}(k) + \tilde{\Gamma}(k)] \tilde{C}(k) = \rho \tilde{C}(k) \tilde{C}(k) [I - \rho \tilde{C}(k)]^{-1}. \quad (11)$$

In these equations $\tilde{\Gamma}(k)$, $\tilde{C}(k)$ are symmetric matrices with elements $\tilde{\gamma}_{ij}(k)$, $\tilde{c}_{ij}(k)$ and I is the unit matrix. Orthonormality allows the easy inversion of Eq. (9) as

$$\tilde{\gamma}_{ij}(k) = \int d\sigma_1 d\sigma_2 f(\sigma_1) f(\sigma_2) \tilde{\gamma}(k, \sigma_1, \sigma_2) p_i(\sigma_1) p_j(\sigma_2). \quad (12)$$

Similar expansions and inversions hold for functions in r space.

With the substitution of the J_0 transforms (6) and (7) for the corresponding sine transforms, these ingredients for a polydisperse fluid in two dimensions are identical to those of a polydisperse fluid in three dimensions¹⁶ and can be solved

with the same numerical procedures. The new feature, the Hankel transform, is evaluated using an orthogonality-preserving algorithm.¹⁷

The generalized pair distribution function

$$\begin{aligned} g(r, \sigma_1, \sigma_2) &= \exp[-\beta \phi(r, \sigma_1, \sigma_2)] \\ &\quad + \gamma(r, \sigma_1, \sigma_2) + b(r, \sigma_1, \sigma_2) \end{aligned} \quad (13)$$

is finally constructed from the self-consistent solution of the (OZ+closure) equations for the coefficients $\gamma_{ij}(r)$. The thermodynamic quantities then directly computable from g are the internal energy U ,

$$\begin{aligned} \frac{\beta U}{N} &= \frac{1}{2} \rho \int d\mathbf{r} d\sigma d\sigma' f(\sigma) f(\sigma') \\ &\quad \times g(r, \sigma, \sigma') \beta \phi(r, \sigma, \sigma'), \end{aligned} \quad (14)$$

and the pressure p ,

$$\begin{aligned} \frac{\beta p}{\rho} &= 1 - \frac{1}{4} \rho \int d\mathbf{r} d\sigma d\sigma' f(\sigma) f(\sigma') \\ &\quad \times g(r, \sigma, \sigma') r \frac{d\beta \phi(r, \sigma, \sigma')}{dr}. \end{aligned} \quad (15)$$

In addition, the isothermal compressibility K_T ,

$$\begin{aligned} \frac{1}{\rho k_B T K_T} &\equiv \beta \left(\frac{\partial p}{\partial \rho} \right)_T \\ &= 1 - \rho \int d\mathbf{r} d\sigma d\sigma' f(\sigma) f(\sigma') c(r, \sigma, \sigma') \\ &= 1 - \rho \tilde{c}_{00}(0), \end{aligned} \quad (16)$$

is obtained from the direct correlation function.

Pair functions of interest can be expressed directly in terms of the computed coefficients. In particular, the number-number pair distribution function and the number-number structure factor¹⁸ are, respectively,

$$g_{NN}(r) \equiv \int d\sigma_1 d\sigma_2 f(\sigma_1) f(\sigma_2) g(r, \sigma_1, \sigma_2) = g_{00}(r), \quad (17)$$

$$\begin{aligned} S_{NN}(k) &\equiv \int d\sigma_1 d\sigma_2 [f(\sigma_1) \delta(\sigma_1 - \sigma_2) \\ &\quad + \rho f(\sigma_1) f(\sigma_2) \tilde{h}(k, \sigma_1, \sigma_2)] = 1 + \rho \tilde{h}_{00}(k). \end{aligned} \quad (18)$$

Further, low order coefficients of $g(r, \sigma_1, \sigma_2)$ can be given a physical interpretation. Thus, local fluctuations in density and size may be expressed in normalized form as

$$\delta \rho_0(\mathbf{r}) = \frac{1}{\rho} \left(\sum_{j=1}^N \delta(\mathbf{r} - \mathbf{r}_j) - \rho \right), \quad (19)$$

$$\delta \rho_1(\mathbf{r}) = \frac{1}{\bar{\sigma} \rho s_\sigma} \left(\sum_{j=1}^N \sigma_j \delta(\mathbf{r} - \mathbf{r}_j) - \bar{\sigma} \rho \right). \quad (20)$$

Their spatial correlations are then given by