

a straightforward extension to the iterative procedure given in Ref. [58] and numerical techniques similar to those described in Ref. [59]. The θ - and ϕ -grids are defined on $[0, \pi/2]$ and $[0, 2\pi]$ respectively. The θ -grid is divided into 200 equal steps on $[0, \pi/8]$, where the ODF changes most rapidly in the nematic phase and into 50 equal steps on $[\pi/8, \pi/2]$ where the ODF is almost zero. The ϕ -grid is divided into 200 equally spaced intervals on $[0, 2\pi]$. We start the iteration with two initial trial distributions, for example a normalized Gaussian $(c/\pi^2) \exp[-2c^2\theta^2/\pi]$ or a constant distribution $1/4\pi$. The choice of the constant distribution is more efficient at low densities where the system is expected to be isotropic. These guesses are substituted into the right hand sides of Eqs. (29) and (30) to obtain a new pair of ODFs, $\Psi_{i,\text{new}}(\theta)$. This procedure is repeated until $\max |\Psi_{i,\text{new}}(\theta) - \Psi_{i,\text{old}}(\theta)| < t$, $i = 1, 2$, where t is the tolerance given by the magnitude of the largest acceptable deviation to the ODF of the previous step: $\Psi_{i,\text{old}}(\theta)$. We set $t = 10^{-9}$. For FMT the solutions take a longer time to converge than for Onsager theory, as each step has a slower execution time due to the increased complexity of the coupled equations (29) and (30).

F. Conditions for Phase Coexistence

Once we have found the ODFs we solve the phase coexistence equations. The requirements for phase coexistence between two phases A and B are the mechanical and chemical equilibria between the phases as well as the equality of temperature in the two coexisting phases (which is trivial in hard-body systems). Hence we have the non-trivial conditions

$$p^A = p^B \quad (31)$$

and

$$\mu_i^A = \mu_i^B, \quad (32)$$

where $i = 1, 2$ again labels the species. We calculate the the total Helmholtz free energy F numerically by inserting $\Psi_i(\theta)$ into Eqs. (5), (13) and (27). Likewise, the pressure can be obtained numerically as

$$p = -\frac{F}{V} + \sum_{i=1}^2 \rho_i \frac{\partial(F/V)}{\partial \rho_i} \quad (33)$$

and the chemical potentials as

$$\mu_i = \frac{\partial(F/V)}{\partial \rho_i}. \quad (34)$$