MONTE CARLO METHODS FOR ESTIMATING INTERFACIAL FREE ENERGIES AND LINE TENSIONS

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Abstract

The surface free energy of (spherical) droplets (bubbles) is obtained by a thermodynamic method for three models (Ising model, binary symmetric Lennard Jones mixture, simple Lennard-Jones fluid). It is shown that for the symmetric models the surface free energy $\gamma(R)$ for the symmetric models behaves as $\gamma(\infty)/\gamma(R) = 1 + (\ell/R)^2$, R being the droplet radius and ℓ a microscopic length. For the LJ fluid, an additional (small) Tolman correction is found. From a corresponding analysis of wall-attached droplets, using $\gamma(R)$ and independently obtained contact angles as an input, estimates for the line tension are inferred. For the binary LJ mixture, which shows a 1st order wetting transition, it is found that the line tension is negative for large contact angles θ but becomes positive for $\theta \approx 30^o$, in good agreement with density functional predictions.