Computation of Mean Field

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1 Introduction

The small magnitude of $\frac{T_c - T^*}{T_c}$, where T_c is the nematic-isotropic phase transition temperature and T^* denotes the virtual transition temperature, has been a long-standing puzzle in the physics of liquid crystals. Extending the mean field theory to include the isotropic, density dependent component of the molecular interaction the magnitudes of both $\frac{T_c - T^*}{T_c}$ and the density change at the transition automatically become in accord with the experimental values. In addition, the value of $\frac{dTc}{dp}$, where p denotes pressure, that is on the same order as the experiment.

This is an excerpt of the Research Article by Ruibao Tao and Ping Sheng, titled "Nematic - Isotropic Phase Transition: An Extended Mean Field Theory". In this contribution project, we were asked to compute the Mean Field, $V(x, y)$ from Interaction Potential, V_{12} between two symmetrical rod - like molecules.

Keywords: Phase Transition, Mean Field, Interaction Potential.

2 Calculations

$$\langle\langle V_{12}\rangle\rangle = 12\varepsilon_m[L(y_1)u^{-4}L(y_2) - 2M(y_1)u^{-2}M(y_2)] - \frac{b}{u^n}W(y_1)P_2(x_1)W(y_2)P_2(x_2)$$

where,
$x = \cos\theta, y = (\frac{s}{a})^2, u = (\frac{a}{\sigma})^3$
$L(y) = \mathcal{L}(y) + \mathcal{L}, M(y) = \mathcal{M}(y) + \mathcal{M}(0)$
$\mathcal{L}(y) = l(y) + \frac{l(\frac{y}{2})}{128} + 2\frac{m(\frac{y}{3})}{729}$
$\mathcal{M}(y) = m(y) + \frac{m(\frac{y}{2})}{16} + 2\frac{m(\frac{y}{3})}{27}$

Now, $l(y) = (1 + 12y + 25.2y^2 + 12y^3 + y^4)(1 - y)^{-10} - 1$
$m(y) = (1 + y)(1 - y)^{-4} - 1, P_2(x) = \frac{(3x^2-1)}{2}$

$\therefore \mathcal{L}(y) = (1+12y+25.2y^2+12y^3+y^4)(1-y)^{-10} - 1 + 8(1+6y+6.3y^2+1.5y^3+0.0625y^4)(2-y)^{-10}) - \frac{1}{128} + 162(1+4y+2.83y^2+0.44y^3+0.004y^4)(3-y)^{-10} - \frac{2}{729}$

$\mathcal{M}(y) = (1 + y)(1 - y)^{-4} - 1 + (2 + y)(2 - y)^{-4} - \frac{1}{16} + 2(3 + y)(3 - y)^{-4} - \frac{2}{27}$

After Simplifying the constant terms we get :-
$\mathcal{L}(y) = (1+12y+25.2y^2+12y^3+y^4)(1-y)^{-10}+8(1+6y+6.3y^2+1.5y^3+0.0625y^4)(2-y)^{-10}+162(1+4y+2.83y^2+0.44y^3+0.004y^4)(3-y)^{-10}-1.010$

$\mathcal{M}(y) = (1+y)(1-y)^{-4}+\frac{(2+y)(2-y)^{-4}}{2}+2(3+y)(3-y)^{-4}-1.136$

Now:- $\mathcal{L}(0)=0, \mathcal{M}(0)=0$
$\therefore L(y)=\mathcal{L}(y)$ and $M(y)=\mathcal{M}(y)$
$W(y)=L(y)$ if $n=12$ and $W(y)=M(y)$ if $n=6$
Now:- $\beta V(x,y)=\sum_{i=1}^{3}\alpha_i\bar{\xi_i}\xi_i(x,y)$

$\xi_1=L(y), \xi_2=M(y), \xi_3=W(y)P_2(x)$
$V(x,y)=kT\sum_{i=1}^{3}\alpha_i\bar{\xi_i}\xi_i(x,y)$
$\bar{\xi_1}=\frac{1}{c}\int_0^c L(y)dy=\frac{15.17879}{0.30544413}=49.6941617$
$\bar{\xi_2}=\frac{1}{c}\int_0^c M(y)dy=\frac{0.498379}{0.30544413}=1.63165355$
$\bar{\xi_3}=\frac{1}{c}\int_0^1\int_0^c W(y)P_2(x)dydx$
$\bar{\xi_3}=\frac{1}{c}\int_0^1\int_0^c M(y)P_2(x)dydx$ (For n = 6)
$\bar{\xi_3}=\frac{1}{c}\times 0.498379\times\int_0^1 P_2(x)dx=0$
$\therefore V(x,y)=kT(\alpha_1\times 49.694L(y)+\alpha_2\times 1.631M(y)+0)$
So,
$V(x,y)=kT(\frac{12\times 49.694L(y)}{u^4\zeta}+\frac{24\times 1.631M(y)}{u^2\zeta})$
$V(x,y)=10^{-23}(\frac{822.932L(y)}{u^4\zeta}+\frac{54.018M(y)}{u^2\zeta})$

3 References

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