Commun. Theor. Phys. (Beijing, China) **42** (2004) pp. 453–458

Vol. 42, No. 3, September 15, 2004

Studies on Nematic Liquid Crystal Using Spin Wave Theory*

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(Received December 22, 2003)

Abstract *A spin wave theory is proposed to study nematic liquid crystals. Since the orientation of the molecular long axis and the angular momentum of the molecule rotating around its long axis have the same direction, operators can be introduced to research the nematic liquid crystal. By transforming the intermolecular interaction potential, the Hamiltonian of the system has the same form as that of the ferromagnetic substance. The relation of the order parameters to the reduced temperature can be obtained. It is in good agreement with the experimental results in the low temperature region. In the high temperature region close to the transition point, by using the Hamiltonian, the transition point can be obtained, which is near to the Maier–Saupe's result.*

PACS numbers: 61.30.Cz, 64.70.Md
Key words: nematic liquid crystals, spin wave, order parameters

1 Introduction

Liquid crystal is essentially a kind of classical fluid. Up to now, its quantum effects have not been found, so classical theories have been used widely, such as L. Onsager molecular field theory,[1] Landau–de Gennes theory,[2,3] and Maier–Saupe molecular field theory.[4,5] Many quite effective methods have been developed in solid-state quantum theory, by which many problems have been solved successfully. For example, ferromagnetic spin wave theory is successful in solving the relation between spontaneous magnetization and temperature in the low temperature region for ferromagnetic substance.[6] We believe that quantum theory can be applied to nematic liquid crystal, too. The spin wave theory is adopted to research the nematic liquid crystal in this paper.

Spin wave theory[7,8] was proposed in 1930 by Bloch. Spin wave is also called magnon, which is a kind of significant elementary excitations in solid-state theory arising from the interactions between local spins. For a spin system composed of N lattice points, only considering the exchange interactions of the nearest neighbor lattices and assuming that the exchange integral J is the same, the interaction of the spins can be expressed as $V=-2J\sum\limits_{(i,j)}\hat{\vec{S}}_i\cdot\hat{\vec{S}}_j=-2\sum\limits_{(i,j)}V_{ij}$, where $\sum\limits_{(i,j)}$ denotes that the sum is over all the nearest pairs of molecules. That is Heisenberg's exchange model.[8,9]

2 Theoretical Model

2.1 *Intermolecular Interaction Potential*

For the rod-like nematic molecules, only considering the interactions of the nearest neighbors, the interaction potential between the i-th and the j-th molecules can be expressed as

$$\begin{aligned}V_{ij}&=U(r_{ij})\mathrm{P}_2(\cos\theta_{ij})=U(r_{ij})\mathrm{P}_2(\vec{\Omega}_i\cdot\vec{\Omega}_j)\\&=U(r_{ij})\Big(\frac{3}{2}\cos^2\theta_{ij}-\frac{1}{2}\Big)\,,\end{aligned}\tag{1}$$

where $U(r_{ij})$ is only related to the molecular center-of-mass position, so it is called the position distribution function, $\mathrm{P}_2(\cos\theta_{ij})$ is the second Legendre polynomial, only related to the molecular orientation, $\vec{\Omega}_i$ and $\vec{\Omega}_j$ are orientation unit vectors of the molecule i and j respectively, and θ_{ij} is the included angle between $\vec{\Omega}_i$ and $\vec{\Omega}_j$.

Usually, the order parameter tensor is defined as

$$Q=\begin{pmatrix}\big\langle\frac{3}{2}\Omega_x^2-\frac{1}{2}\big\rangle & \big\langle\frac{3}{2}\Omega_x\Omega_y\big\rangle & \big\langle\frac{3}{2}\Omega_x\Omega_z\big\rangle\\ \big\langle\frac{3}{2}\Omega_y\Omega_x\big\rangle & \big\langle\frac{3}{2}\Omega_y^2-\frac{1}{2}\big\rangle & \big\langle\frac{3}{2}\Omega_y\Omega_z\big\rangle\\ \big\langle\frac{3}{2}\Omega_z\Omega_x\big\rangle & \big\langle\frac{3}{2}\Omega_z\Omega_y\big\rangle & \big\langle\frac{3}{2}\Omega_z^2-\frac{1}{2}\big\rangle\end{pmatrix}.\tag{2}$$

Using additive formula of spherical function:

$$\begin{aligned}\mathrm{P}_l(\cos\theta_{ij})&=\mathrm{P}_l(\cos\theta_i)\mathrm{P}_l(\cos\theta_j)\\&\quad+2\sum_{m=1}^{l}\frac{(l-m)!}{(l+m)!}\mathrm{P}_l^m(\cos\theta_i)\mathrm{P}_l^m(\cos\theta_j)\\&\quad\times\cos[m(\varphi_i-\varphi_j)]\,,\end{aligned}\tag{3}$$

where

$$\begin{aligned}&\cos\theta_{ij}=\cos\theta_i\cos\theta_j+\sin\theta_i\sin\theta_j\cos(\varphi_i-\varphi_j)\,,\\&\Omega_x=\sin\theta\cos\varphi\,,\ \ \Omega_y=\sin\theta\sin\varphi\,,\ \ \Omega_z=\cos\theta\,.\end{aligned}$$

Substituting Eq. (3) into Eq. (1), we have

$$V_{ij}=U(r_{ij})\frac{2}{3}\sum_{\mu\nu}Q_{\mu\nu}(i)Q_{\mu\nu}(j)\,.\tag{4}$$

*The project supported by the Natural Science Foundation of Hebei Province of China under Grant No. A2004000140 and the Natural Science Foundation of Hebei Education Committee under Grant No. 2003107

2.2 *Operator Expression of Order Parameter Tensor*

Nematic phase is characterized by a high degree of long range orientational order, the molecules' spontaneous order with their long axes roughly parallel. For the rigid rod-like molecule, the direction of the molecule's long axis is defined as orientation $\vec{\Omega}$. Because the molecule rotates around its long axis, the direction of angular momentum $\vec{L}$ also lies along the long axis. Therefore $\vec{\Omega}$ and $\vec{L}$ have the same direction, as shown in Fig. 1. We define orientation operator

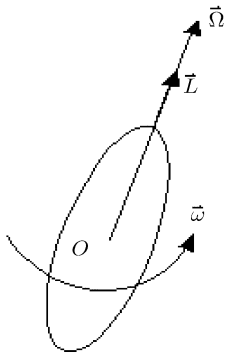

Fig. 1 Sketch of the rod-like molecule.

$$\vec{\Omega} = \frac{\hat{\vec{L}}}{|\vec{L}|} = \frac{\hat{\vec{L}}}{\sqrt{l(l+1)}\hbar}\,, \tag{5}$$

$$\hat{\Omega}_x = \frac{\hat{L}_x}{\sqrt{l(l+1)}\hbar}, \qquad \hat{\Omega}_y = \frac{\hat{L}_y}{\sqrt{l(l+1)}\hbar}\,,$$

$$\hat{\Omega}_z = \frac{\hat{L}_z}{\sqrt{l(l+1)}\hbar}\,. \tag{6}$$

In this way, unit vector $\vec{\Omega}$ can be expressed as the form of operator, which is very crucial in our theory. Then solid-state quantum theory can be used to research nematic liquid crystal. Substituting Eq. (6) into Eq. (2), Q can be written as

$$Q = \frac{1}{l(l+1)\hbar^2}\begin{pmatrix} \frac{3}{2}\hat{L}_x^2 - \frac{1}{2}l(l+1)\hbar^2 & \frac{3}{2}\hat{L}_x\hat{L}_y & \frac{3}{2}\hat{L}_x\hat{L}_z \\ \frac{3}{2}\hat{L}_y\hat{L}_x & \frac{3}{2}\hat{L}_y^2 - \frac{1}{2}l(l+1)\hbar^2 & \frac{3}{2}\hat{L}_y\hat{L}_z \\ \frac{3}{2}\hat{L}_z\hat{L}_x & \frac{3}{2}\hat{L}_z\hat{L}_y & \frac{3}{2}\hat{L}_z^2 - \frac{1}{2}l(l+1)\hbar^2 \end{pmatrix}. \tag{7}$$

Making Eq. (7) symmetric, we have

$$Q = \frac{1}{l(l+1)\hbar^2}\begin{pmatrix} \frac{3}{2}\hat{L}_x^2 - \frac{1}{2}l(l+1)\hbar^2 & \frac{3}{4}(\hat{L}_x\hat{L}_y + \hat{L}_y\hat{L}_x) & \frac{3}{4}(\hat{L}_x\hat{L}_z + \hat{L}_z\hat{L}_x) \\ \frac{3}{4}(\hat{L}_y\hat{L}_x + \hat{L}_x\hat{L}_y) & \frac{3}{2}\hat{L}_y^2 - \frac{1}{2}l(l+1)\hbar^2 & \frac{3}{4}(\hat{L}_y\hat{L}_z + \hat{L}_z\hat{L}_y) \\ \frac{3}{4}(\hat{L}_z\hat{L}_x + \hat{L}_x\hat{L}_z) & \frac{3}{4}(\hat{L}_z\hat{L}_y + \hat{L}_y\hat{L}_z) & \frac{3}{2}\hat{L}_z^2 - \frac{1}{2}l(l+1)\hbar^2 \end{pmatrix}. \tag{8}$$

Then,

$$Q_{\mu\nu} = \begin{cases} \dfrac{1}{l(l+1)\hbar^2}\dfrac{3}{4}(\hat{L}_\mu\hat{L}_\nu + \hat{L}_\nu\hat{L}_\mu), & \mu \neq \nu, \\ \dfrac{1}{l(l+1)\hbar^2}\Big[\dfrac{3}{2}\hat{L}_\mu^2 - \dfrac{1}{2}l(l+1)\hbar^2\Big], & \mu = \nu; \quad \mu,\nu = 1,2,3\,. \end{cases} \tag{9}$$

Obviously, as it is shown in the definition Eq. (9), the order parameter tensor is symmetric and traceless, i.e. $\hat{Q}_{\mu\nu} = \hat{Q}_{\nu\mu}$, $\mathrm{Tr}\ Q = 0$.

2.3 $\vec{T}$ *Vector and* $\vec{\tau}$ *Vector and Their Operator Expression*

Because the order parameter tensor Q is a symmetric and traceless two-order tensor, it can be denoted by a five-dimensional vector $\vec{T}$ as

$$T_1 = \sqrt{\frac{3}{2}}Q_{33}, \quad T_2 = \sqrt{\frac{1}{2}}(Q_{11} - Q_{22}), \quad T_3 = \sqrt{2}Q_{12}, \quad T_4 = \sqrt{2}Q_{23}, \quad T_5 = \sqrt{2}Q_{31}\,. \tag{10}$$

It also can be written in a matrix form,

$$\vec{T} = \begin{pmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \end{pmatrix}, \quad \vec{T}^\dagger = \begin{pmatrix} {T_1}^* & {T_2}^* & {T_3}^* & {T_4}^* & {T_5}^* \end{pmatrix}. \tag{11}$$

Such a definition can satisfy the equation $\sum_{i=1}^{5} {T_i}^2 = \sum_{\mu\nu} Q_{\mu\nu}Q_{\mu\nu} = \vec{T}^{\dagger}\cdot\vec{T}$, thus equation (4) can be written as

$$V_{ij} = U(r_{ij})\frac{2}{3}\vec{T}(i)\cdot\vec{T}(j)\,. \tag{12}$$

From Eqs. (9) and (10), the operator expression of $\vec{T}$ can be obtained as

$$\begin{aligned}
&\hat{T}_1 = \frac{\sqrt{3/2}[3\hat{L}_z{}^2 - l(l+1)\hbar^2]/2}{l(l+1)\hbar^2}, \quad \hat{T}_2 = \frac{3\sqrt{1/2}(\hat{L}_x^2 - \hat{L}_y^2)/2}{l(l+1)\hbar^2}, \quad \hat{T}_3 = \frac{3\sqrt{2}(\hat{L}_x\hat{L}_y + \hat{L}_y\hat{L}_x)/4}{l(l+1)\hbar^2}\,,\\
&\hat{T}_4 = \frac{3\sqrt{2}(\hat{L}_y\hat{L}_z + \hat{L}_z\hat{L}_y)/4}{l(l+1)\hbar^2}, \quad \hat{T}_5 = \frac{3\sqrt{2}(\hat{L}_z\hat{L}_x + \hat{L}_x\hat{L}_z)/4}{l(l+1)\hbar^2}\,.
\end{aligned} \tag{13}$$

We introduce step operators $\hat{L}_{\pm} = \hat{L}_x \pm \mathrm{i}\hat{L}_y$. For convenience, the origin of coordinates is chosen at the molecular center-of-mass, and then we can get some commutation relations

$$\begin{aligned}
&[\hat{L}_x, \hat{L}_y] = -\mathrm{i}\hbar\hat{L}_z, \quad [\hat{L}_z, \hat{L}_{\pm}] = \mp\hbar\hat{L}_{\pm}, \quad [\hat{L}_+, \hat{L}_-] = -2\hbar\hat{L}_z, \quad \hat{L}_{\pm}\hat{L}_{\mp} = \hat{L}^2 - \hat{L}_z^2 \mp \hbar\hat{L}_z\,,\\
&\hat{L}_x\hat{L}_y + \hat{L}_y\hat{L}_x = \frac{1}{2\mathrm{i}}(\hat{L}_+^2 - \hat{L}_-^2), \quad \hat{L}_x^2 - \hat{L}_y^2 = \frac{1}{2}(\hat{L}_+^2 + \hat{L}_-^2), \quad \hat{L}_x = \frac{1}{2}(\hat{L}_+ + \hat{L}_-), \quad \hat{L}_y = \frac{1}{2\mathrm{i}}(\hat{L}_+ - \hat{L}_-)\,.
\end{aligned} \tag{14}$$

For $\hat{\vec{T}}$ cannot directly operate on the eigenstate of $\hat{L}_z$, we define $\hat{\vec{\tau}}$

$$\hat{\tau}_0 = \hat{T}_1, \quad \hat{\tau}_{-1} = \frac{1}{\sqrt{2}}(-\mathrm{i}\hat{T}_4 + \hat{T}_5) = \frac{3(\hat{L}_z\hat{L}_- + \hat{L}_-\hat{L}_z)/4}{l(l+1)\hbar^2} = \hat{\tau}_{+1}^*, \quad \hat{\tau}_{-2} = \frac{1}{\sqrt{2}}(\hat{T}_2 + \mathrm{i}\hat{T}_3) = \frac{3\sqrt{1/2}\hat{L}_+^2/4}{l(l+1)\hbar^2} = \hat{\tau}_{+2}^*\,. \tag{15}$$

Such the definition can satisfy the equation $\hat{\vec{\tau}}^{\dagger}\cdot\hat{\vec{\tau}} = \hat{\vec{T}}^{\dagger}\cdot\hat{\vec{T}}$, thus equation (12) can be written as

$$\begin{aligned}
V_{ij} &= U(r_{ij})\frac{2}{3}[\hat{\tau}(i)]^{\dagger}[\hat{\tau}(j)]\\
&= \frac{2}{3}U(r_{ij})\big(\hat{\tau}_{-2}^*(i)\ \hat{\tau}_{-1}^*(i)\ \hat{\tau}_0^*(i)\ \hat{\tau}_{+1}^*(i)\ \hat{\tau}_{+2}^*(i)\big)\begin{pmatrix}\hat{\tau}_{-2}(j)\\ \hat{\tau}_{-1}(j)\\ \hat{\tau}_0(j)\\ \hat{\tau}_{+1}(j)\\ \hat{\tau}_{+2}(j)\end{pmatrix}\\
&= \frac{2}{3}U(r_{ij})\big[\hat{\tau}_{+2}(i)\hat{\tau}_{-2}(j) + \hat{\tau}_{+1}(i)\hat{\tau}_{-1}(j) + \hat{\tau}_0(i)\hat{\tau}_0(j) + \hat{\tau}_{-1}(i)\hat{\tau}_{+1}(j) + \hat{\tau}_{-2}(i)\hat{\tau}_{+2}(j)\big]\,.
\end{aligned} \tag{16}$$

Supposing $\{|l, m_i\rangle|l, m_j\rangle\}$ is a set of eigenvectors in $(\hat{L}^2, \hat{L}_z)$ representation, using $\hat{L}_z|l,m\rangle = m\hbar|l,m\rangle$, $\hat{L}_{\pm}|l,m\rangle = \hbar C_{\pm}^{lm}|l, m\mp 1\rangle$, $C_{\pm}^{lm} = [(l\pm m)(l\mp m+1)]^{1/2}$, we have

$$\begin{aligned}
&\hat{\tau}_0|l,m\rangle = \frac{\sqrt{3/2}[3m^2/2 - (l+1)/2]}{l(l+1)}|l,m\rangle, \quad \hat{\tau}_{-1}|l,m\rangle = \frac{3}{4}\frac{(2m+1)C_-^{lm}}{l(l+1)}|l,m+1\rangle\,,\\
&\hat{\tau}_{+1}|l,m\rangle = \frac{3}{4}\frac{(2m-1)C_+^{lm}}{l(l+1)}|l,m-1\rangle, \quad \hat{\tau}_{-2}|l,m\rangle = \frac{3\sqrt{1/2}C_-^{lm}C_-^{l,m+1}/2}{l(l+1)}|l,m+2\rangle\,,\\
&\hat{\tau}_{+2}|l,m\rangle = \frac{3\sqrt{1/2}C_+^{lm}C_+^{l,m-1}/2}{l(l+1)}|l,m-2\rangle\,.
\end{aligned} \tag{17}$$

2.4 *Holstein–Primakoff Transformation*

$|l,m\rangle$ represents single particle state, where l is invariable, m is variable. Let $n = l - m$, then single particle state can also be expressed as $|n\rangle = |l, l-n\rangle$. Introducing creation operator and annihilation operator

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle, \quad \hat{a}^{\dagger}|n\rangle = \sqrt{n+1}|n+1\rangle, \quad [\hat{a}, \hat{a}^{\dagger}] = 1, \quad \hat{a}^{\dagger}\hat{a}|n\rangle = n|n\rangle\,, \tag{18}$$

where $\hat{a}^{\dagger}$ is a quasi-particle creation operator, $\hat{a}$ is a quasi-particle annihilation operator, $\hat{a}^{\dagger}\hat{a}$ is a quasi-particle number operator. The spin wave is a quasi-particle and Boson. Applying these operators to single particle state, we have

$$\begin{aligned}
&\hat{a}|n\rangle = \hat{a}|l, l-n\rangle = \hat{a}|l,m\rangle = \sqrt{l-m}|l, l-(n-1)\rangle = \sqrt{l-m}|l,m+1\rangle\,,\\
&\hat{a}^{\dagger}|n\rangle = \hat{a}^{\dagger}|l, l-n\rangle = \hat{a}^{\dagger}|l,m\rangle = \sqrt{l-m+1}|l, l-(n+1)\rangle = \sqrt{l-m+1}|l,m-1\rangle\,.
\end{aligned} \tag{19}$$

So $\hat{\vec{\tau}}$ can be expressed by $\hat{a}^\dagger$ and $\hat{a}$,

$$\hat{\tau}_0 = \frac{1}{2}\sqrt{\frac{3}{2}}\frac{1}{l(l+1)}[l(2l-1)-3(2l-\hat{a}^\dagger\hat{a})\hat{a}^\dagger\hat{a}], \quad \hat{\tau}_{-1} = \frac{3}{4}\frac{2l-1-2\hat{a}^\dagger\hat{a}}{l(l+1)}\sqrt{2l-\hat{a}^\dagger\hat{a}}\hat{a}\,,$$
$$\hat{\tau}_{+1} = \frac{3}{4}\frac{2l+1-2\hat{a}^\dagger\hat{a}}{l(l+1)}\sqrt{2l-\hat{a}^\dagger\hat{a}+1}\hat{a}^\dagger, \quad \hat{\tau}_{-2} = \frac{3}{2}\sqrt{\frac{1}{2}}\frac{1}{l(l+1)}\sqrt{2l-\hat{a}^\dagger\hat{a}-1}\sqrt{2l-\hat{a}^\dagger\hat{a}}\hat{a}\hat{a}\,,$$
$$\hat{\tau}_{+2} = \frac{3}{2}\sqrt{\frac{1}{2}}\frac{1}{l(l+1)}\sqrt{2l-\hat{a}^\dagger\hat{a}+2}\sqrt{2l-\hat{a}^\dagger\hat{a}+1}\hat{a}^\dagger\hat{a}^\dagger\,. \tag{20}$$

If $l \gg 1$ (This estimation can be proved as follows. For $\vec{L} = I\vec{\omega}$, rotational kinetic energy can be expressed as $\overline{I\omega^2/2} = k_BT/2$. So $\overline{L^2} = Ik_BT$, $\overline{l(l+1)\hbar^2} = Ik_BT$. Using approximation, when l is comparative large, the formula can be approximated as $\bar{l} = (Ik_BT)^{1/2}/\hbar$. For nematic liquid crystal molecules $I = 10^{-43} \sim 10^{-46}\mathrm{kg}\cdot\mathrm{m}^2$, taking numerical estimation we can get $l \approx 10 \sim 10^2$ under the condition of room temperature. So the assumption $l \gg 1$ is reasonable.), we have $n/l \ll 1$, and $\hat{\tau}_k$ can be approximately expressed as

$$\hat{\tau}_0 \approx \frac{1}{2}\sqrt{\frac{3}{2}}\frac{1}{l^2}[2l^2-6l\hat{a}^\dagger\hat{a}+3(\hat{a}^\dagger\hat{a})^2] \approx \sqrt{\frac{3}{2}}\frac{1}{l}(l-3\hat{a}^\dagger\hat{a})\,,$$
$$\hat{\tau}_{-1} \approx \frac{3}{4}\frac{(2l-1)\sqrt{2l}}{l(l+1)}\Big[1-\Big(\frac{1}{4l}+\frac{2}{2l-1}\Big)\hat{a}^\dagger\hat{a}\Big]\hat{a} \approx \frac{3}{\sqrt{2l}}\hat{a}, \quad \hat{\tau}_{+1} \approx \frac{3}{\sqrt{2l}}\Big[1-\frac{5}{2}\frac{2}{2l+1}\hat{a}^\dagger\hat{a}\Big]\hat{a}^\dagger \approx \frac{3}{\sqrt{2l}}\hat{a}^\dagger\,,$$
$$\hat{\tau}_{-2} \approx \sqrt{\frac{1}{2}}\frac{3}{l}\hat{a}\hat{a}, \quad \hat{\tau}_{+2} \approx \sqrt{\frac{1}{2}}\frac{3}{l}\hat{a}^\dagger\hat{a}^\dagger\,. \tag{21}$$

Intermolecular interaction potential function Eq. (16) can be expressed with the creation operator and the annihilation operator as follows:

$$\begin{aligned} V_{ij} &= U(r_{ij})\frac{2}{3}[\hat{\tau}_{+2}(i)\hat{\tau}_{-2}(j)+\hat{\tau}_{+1}(i)\hat{\tau}_{-1}(j)+\hat{\tau}_0(i)\hat{\tau}_0(j)+\hat{\tau}_{-1}(i)\hat{\tau}_{+1}(j)+\hat{\tau}_{-2}(i)\hat{\tau}_{+2}(j)] \\ &= U(r_{ij})\frac{2}{3}\Big[\frac{9}{2l^2}(\hat{a}_i^\dagger\hat{a}_i^\dagger\hat{a}_j\hat{a}_j+\hat{a}_i\hat{a}_i\hat{a}_j^\dagger\hat{a}_j^\dagger)+\frac{9}{2l}(\hat{a}_i^\dagger\hat{a}_j+\hat{a}_i\hat{a}_j^\dagger)+\frac{3}{2l^2}(l-3\hat{a}_i^\dagger\hat{a}_i)(l-3\hat{a}_j^\dagger\hat{a}_j)\Big] \\ &\approx U(r_{ij})\frac{2}{3}\Big[\frac{9}{2l}(\hat{a}_i^\dagger\hat{a}_j+\hat{a}_i\hat{a}_j^\dagger)+\frac{3}{2l}(l-3\hat{a}_i^\dagger\hat{a}_i-3\hat{a}_j^\dagger\hat{a}_j)\Big]\,. \end{aligned} \tag{22}$$

3 System Hamiltonian in Cell Model

The cell model of liquid[10−12] is adopted in our theory. The region of liquid crystal is divided into N small regions, and every small region is regarded as a cell. The centers of the cells constitute the spatial lattice. The molecules are restricted to be on a simple-cubic lattice and to interact only with their nearest neighbors, and the Hamiltonian of the system can be written as

$$\begin{aligned} \hat{H}_0 &\approx \frac{1}{2}U(r_{ij})\frac{2}{3}\sum_{i,\delta}{}'\Big[\frac{9}{2l}(\hat{a}_i^\dagger\hat{a}_{i+\delta}+\hat{a}_i\hat{a}_{i+\delta}^\dagger)+\frac{3}{2l}(l-3\hat{a}_i^\dagger\hat{a}_i-3\hat{a}_{i+\delta}^\dagger\hat{a}_{i+\delta})\Big] \\ &= \frac{1}{2}ZNU(r_{ij})-3\frac{U(r_{ij})}{l}Z\sum_i\hat{a}_i^\dagger\hat{a}_i+\frac{3U(r_{ij})}{2l}\sum_{i,\delta}{}'(\hat{a}_i^\dagger\hat{a}_{i+\delta}+\hat{a}_i\hat{a}_{i+\delta}^\dagger)\,, \end{aligned} \tag{23}$$

where we suppose that the molecules between two lattices have the same $U(r_{ij})$; the factor $1/2$ is required to avoid counting intermolecular interactions twice, $\sum_{i,\delta}{}'$ represents that the summation is exclusive of the item whose $\delta \neq 0$. Because $U < 0$, replacing U by $-|U|$, then equation (23) can be written as

$$\hat{H}_0 = E_0 + 3Z\frac{|U(r_{ij})|}{l}\sum_i\hat{a}_i^\dagger\hat{a}_i-\frac{3|U(r_{ij})|}{2l}\sum_{i,\delta}{}'(\hat{a}_i^\dagger\hat{a}_{i+\delta}+\hat{a}_i\hat{a}_{i+\delta}^\dagger) \tag{24}$$

where $E_0 = -ZN|U(r_{ij})|/2$. The Hamiltonian of ferromagnetic spin wave theory was reported as[8]

$$\hat{H}_0 = -ZN|J|S^2+2Z|J|S\sum_l\hat{a}_l^\dagger\hat{a}_l-|J|S\sum_{l,\delta}{}'(\hat{a}_l^\dagger\hat{a}_{l+\delta}+\hat{a}_l\hat{a}_{l+\delta}^\dagger)\,. \tag{25}$$

It is clear that the forms of Eqs. (24) and (25) are in good agreement. Transferring Eq. (24) from coordinate space to momentum space, the Hamiltonian can be rewritten as

$$\hat{H}_0 = E_0 + 3Z\frac{|U(r_{ij})|}{l}\sum_i\frac{1}{N}\sum_{k,k'}\mathrm{e}^{\mathrm{i}(\vec{k}-\vec{k}')\cdot\vec{R}_i}\hat{b}_{k'}^\dagger\hat{b}_k$$

$$-\frac{3|U(r_{ij})|}{2l}{\sum_{i,\delta}}'\frac{1}{N}\sum_{k,k'}(\,\mathrm{e}^{-\mathrm{i}\vec{k}'\cdot\vec{R}_i}\,\mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{R}_{i+\delta}}\hat{b}^{\dagger}_{k'}\hat{b}_k+\mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{R}_i}\,\mathrm{e}^{-\mathrm{i}\vec{k}\cdot\vec{R}_{i+\delta}}\hat{b}_k\hat{b}^{\dagger}_{k'})$$
$$=E_0+3Z\frac{|U(r_{ij})|}{l}\sum_k(1-\gamma_k)\hat{b}^{\dagger}_k\hat{b}_k=E_0+\sum_k\hbar\omega_k\hat{b}^{\dagger}_k\hat{b}_k\,, \tag{26}$$

where $\gamma_k=(1/Z)\sum_\delta \mathrm{e}^{\mathrm{i}\vec{k}\cdot\delta}=\gamma_{-k}$, and

$$\hbar\omega_k=3Z[|U(r_{ij})|/l](1-\gamma_k)\,.$$

Crystals have the characteristics of inversion symmetry. Different crystals have different γ_k, so the relation between the frequency of spin wave and the wave vector $\vec{k}$ can be calculated by combining the symmetry of the crystal. Under low temperature circumstances, by using long wave condition to expand γ_k, we can solve $\hbar\omega_k$. Because the long wave dispersion relation of SC, BCC, and FCC are the same,[8] we have

$$\hbar\omega_k=3\frac{|U(r_{ij})|}{l}\Big(Z-\sum_\delta \mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{\delta}}\Big)\approx 3\frac{|U(r_{ij})|}{2l}\sum_\delta(\vec{k}\cdot\vec{\delta})^2$$
$$=3\frac{|U(r_{ij})|}{l}a^2k^2\,, \tag{27}$$

where a is the lattice constant of the crystal cell.

4 Results

Choosing z-axis as the preferred direction, then $OZ//\vec{n}$, and from Eq. (2) we have

$$Q=\langle\hat{Q}\rangle_T=\begin{pmatrix}-S/2 & 0 & 0\\ 0 & -S/2 & 0\\ 0 & 0 & S\end{pmatrix}, \tag{28}$$

where S is the order-parameter, and

$$S=\langle\hat{Q}_{33}\rangle=\langle \mathrm{P}_2(\cos\theta)\rangle\,.$$

From $\hat{\tau}_0=\hat{T}_1=\sqrt{3/2}\hat{Q}_{33}$, we can get

$$S=\langle\hat{Q}_{33}\rangle_T=\sqrt{\frac{2}{3}}\langle\hat{\tau}_0\rangle_T$$
$$=\sqrt{\frac{2}{3}}\Big\langle\sqrt{\frac{3}{2}}\frac{1}{l}(l-3\hat{a}^{\dagger}_i\hat{a}_i)\Big\rangle_T$$
$$\approx 1-\frac{3}{8lf}\Big(\frac{k_BTl}{3\pi|U(r_{ij})|}\Big)^{3/2}2.612\approx 1-CT_R^{3/2}\,, \tag{29}$$

where $C=(3/8lf)(l/3\pi)^{3/2}2.612$, $V=Na^3/f$, $T_R=k_BT/|U(r_{ij})|$, and f is the structural coefficient. The relation of Bose–Einstein statistics $\langle\hat{n}_k\rangle=1/(\,\mathrm{e}^{\hbar\omega/k_BT}-1)$ is used in Eq. (29). By numerical calculation, the relation of the order parameters to the reduced temperature can be obtained, which is shown in Fig. 2.

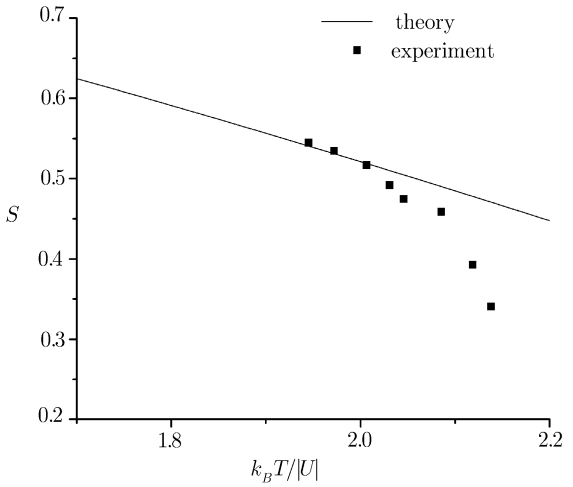

Fig. 2 Nematic order parameter S versus reduced temperature. The solid curve is our result, while squares indicate experimental data of Ref. [13].

5 Discussion

It can be seen from Fig. 2 that the order parameter S decreases as the reduced temperature increases, which denotes that when the temperature increases the order degree of the system is destroyed by heat motion of the molecules. The results obtained by spin wave theory are in good agreement with those of the experiments,[13] especially in the low temperature region. It is the first time that quantum theory is applied to research the nematic liquid crystals. For the review of articles and books dealing with this subject, we may mention that most of the theories about nematic liquid crystals have solved the order problems close to the transition point, but in the low temperature region these theories do not hold. The spin wave theory of nematic liquid crystal can solve the problem. Just as in ferromagnetic theory, in order to discuss the relation between spontaneous magnetization and temperature, the theory of molecular field and high temperature expansion approximation method are adopted in the high temperature region close to the Curie point; spin wave theory is adopted at the low temperature region.[6]

We use the theory of molecular field to calculate the nematic-isotropic transition point in the high temperature region close to the transition point. From Eq. (22), we have

$$\hat{H}=-\frac{1}{2}|U(r_{ij})|\frac{2}{3}\sum_{i\neq j}\{\hat{\tau}_{+2}(i)\hat{\tau}_{-2}(j)+\hat{\tau}_{+1}(i)\hat{\tau}_{-1}(j)+\hat{\tau}_0(i)\hat{\tau}_0(j)+\hat{\tau}_{-1}(i)\hat{\tau}_{+1}(j)+\hat{\tau}_{-2}(i)\hat{\tau}_{+2}(j)\}\,. \tag{30}$$

Equation (30) represents that the system energy is the summation of the molecule interaction potentials. To the i-th molecule, it lies in the potential field created by the $N-1$ molecules, which is called molecular field.[14−17] Substituting $\hat{\tau}_k(j)$ for $\langle\hat{\tau}_k\rangle_T$, which is the statistical average of $\hat{\tau}_k$, we can see that only the statistical average of $\hat{\tau}_0$ is none zero from Eq. (17), and $\langle\hat{\tau}_0\rangle_T = \sqrt{3/2}\,S$, and we have

$$\hat{H} = -\frac{1}{2}|U(r_{ij})|\frac{2}{3}\sum_{i=1}^{N}\{\hat{\tau}_0(i)[Z\langle\hat{\tau}_0\rangle_T]\} = -\frac{1}{2}|U(r_{ij})|\sqrt{\frac{2}{3}}SZ\sum_{i=1}^{N}\hat{\tau}_0(i)\,. \tag{31}$$

Without considering the identity principle of microparticles, the Hamiltonian of single particle can be expressed as

$$\hat{H}_i = -\frac{1}{2}|U(r_{ij})|\frac{2}{3}\sqrt{\frac{3}{2}}SZ\hat{\tau}_0\,, \tag{32}$$

the statistical average of $\hat{\tau}_0$ is

$$\langle\hat{\tau}_0\rangle = \frac{\sum\limits_{m=-l}^{l}\{\sqrt{3/2}[3m^2/2 - l(l+1)/2]/l(l+1)\}\,\mathrm{e}^{-\beta E_m}}{\sum\limits_{m=-l}^{l}\mathrm{e}^{-\beta E_m}}\,, \tag{33}$$

where

$$E_m = -\frac{1}{2}|U(r_{ij})|\frac{2}{3}\sqrt{\frac{3}{2}}SZ\frac{\sqrt{3/2}[3m^2/2 - l(l+1)/2]}{l(l+1)}\,. \tag{34}$$

Defining $\xi = -3Z|U(r_{ij})|/4k_BT$, then

$$S = \frac{\sum\limits_{l=0}^{\infty}\sum\limits_{m=-l}^{l}\{3m^2/2l(l+1) - 1/2\}\,\mathrm{e}^{-\xi Sm^2/l(l+1)}}{\sum\limits_{l=0}^{\infty}\sum\limits_{m=-l}^{l}\mathrm{e}^{-\xi Sm^2/l(l+1)}} = \frac{\sum\limits_{l=0}^{\infty}\sum\limits_{m=-l}^{l}\{[3m^2/2l(l+1)]\,\mathrm{e}^{-\xi Sm^2/l(l+1)}\}}{\sum\limits_{l=0}^{\infty}\sum\limits_{m=-l}^{l}\mathrm{e}^{-\xi Sm^2/l(l+1)}} - \frac{1}{2}\,. \tag{35}$$

Obviously, zero is a solution to Eq. (35), and none zero solution must exist. By numerical calculation, we can obtain that the order parameter is 0.4111 at the transition point, which is close to Maier–Saupe's result 0.4289.[18]

In our model, the items containing products of more than two operators are neglected by using the approximation $n/l \ll 1$ in Eq. (20). If the effects of the higher order items on the energy of the system are considered, it can be anticipated that the theory can solve the problems in the high temperature region close to the transition point. These questions are to be studied in the subsequent work.

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