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Ryan P. ONeill
Old Dominion University

Giangvuthanh Nguyen
Old Dominion University

Xiang Xu
Old Dominion University

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Cover Page Footnote

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Asymptotic Expansion of a Maier-Saupe Type Potential Near the Nematic-Isotropic Transition Point in Liquid Crystals

Giangvuthanh Nguyen[‡1], Ryan Oneill[*2], and Xiang Xu[†1]

[1]Department of Mathematics and Statistics, Old Dominion University, Norfolk, VA 23529.

[2]Department of Physics,Old Dominion University, Norfolk, VA 23529.

Abstract

In this paper we study a Maier-Saupe type bulk potential (Maier & Saupe, 1959) in the Landau-de Gennes free energy in the Q-tensor theory modeling nematic liquid crystal configurations. This potential was originally introduced in Katriel et al. (1986), which is considered as a natural enforcement of a physical constraint on the eigenvalues of symmetric, traceless Q-tensors. More specifically, we present a rigorous derivation of the asymptotic expansion of this singular potential near the nematic-isotropic transition point up to the 4-th order.

1 Introduction

Liquid crystals are a typical type of soft matters that are intermediate between crystalline solids and isotropic fluids. Their anisotropic properties lead to various mechanical, optical and rheological properties that have induced a wide range of commercial applications (De Gennes & Prost, 1993). The simplest phase of liquid crystals is called the nematic phase, where there is a long-range orientational order that makes the molecules almost align parallel to each other, but no correlation to the molecular center of mass positions. Generally speaking, there are two types of models to describe the nematic liquid phase, i.e., the mean field model and the continuum model. In the mean field theory, the local alignment of molecules is described by a probability distribution function on the unit sphere (De Gennes & Prost, 1993; Maier & Saupe, 1959; Virga, 1994). Let $\mathbf{n}$ be a unit vector in $\mathbb{R}^3$ that represents the orientation of a single liquid crystal molecule, and $\rho(x;\mathbf{n})$ be the density distribution function of molecular orientations at a point $x \in \Omega \subset \mathbb{R}^3$. The de Gennes Q-tensor, which is defined to be the deviation of associated second moment of ρ from its isotropic value, reads

$$Q = \int_{\mathbb{S}^2} \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbb{I}_3 \right) \rho(\mathbf{n})\, \mathrm{d}S. \tag{1.1}$$

Since the de Gennes Q-tensor vanishes in the isotropic phase, it is regarded as an order parameter. Meanwhile, it is easy to check from (1.1) that any de Gennes Q-tensor is symmetric, traceless, and all its eigenvalues satisfy the constraint $-1/3 \leq \lambda_i(Q) \leq 2/3$, $1 \leq i \leq 3$. Note that if the smallest eigenvalue of the Q-tensor reaches $-1/3$, then it implies all molecules are pointing on a great circle perpendicular to the associated eigenvector (Virga, 1994), which is physically unrealistic. Therefore, the effective domain of the de Gennes Q-tensor is

$$-\frac{1}{3} < \lambda_i(Q) < \frac{2}{3}, \qquad 1 \leq i \leq 3. \tag{1.2}$$

Alternatively, in the continuum model a phenomenological Landau-de Gennes theory is proposed (Ball, 2012; De Gennes & Prost, 1993; Mottram & Newton, 2014). In this theory the basic element is a symmetric, traceless 3×3 matrix in the so called Q-tensor space (Mottram & Newton, 2014)

$$\mathbb{Q} \stackrel{\text{def}}{=} \left\{ M \in \mathbb{R}^{3\times 3} \,\middle|\, \operatorname{tr}(M) = 0,\, M^T = M \right\}. \tag{1.3}$$

without any eigenvalue constraints. This basic element is at times referred to as the mathematical Q-tensor. In this framework the relevant free energy functional is derived as a nonlinear integral

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functional of the Q-tensor and its spatial derivatives (Ball, 2012):

$$\mathcal{E}[Q] = \int_\Omega \mathcal{F}(Q(x))\,\mathrm{d}x. \tag{1.4}$$

The free energy density functional $\mathcal{F}$ in (1.4) is the sum of the elastic part $\mathcal{F}_{el}$ and the bulk part $\mathcal{F}_{bulk}$ that depends only on Q. One typical form of $\mathcal{F}_{el}$ reads (Ball, 2012; Ball & Majumdar, 2010; Longa et al., 1987)

$$\mathcal{F}_{el} = L_1|\nabla Q|^2 + L_2\partial_j Q_{ik}\partial_k Q_{ij} + L_3\partial_j Q_{ij}\partial_k Q_{ik} + L_4 Q_{lk}\partial_k Q_{ij}\partial_l Q_{ij}. \tag{1.5}$$

Here, $\partial_k Q_{ij}$ represents the k-th spatial derivative of the ij-th component of Q, $L_1,\cdots L_4$ are material dependent constants, and Einstein summation convention over repeated indices is used. The retention of the L_4 cubic term is that it allows complete reduction to the classical Oseen-Frank energy (Hardt et al., 1986) with four elastic terms. This cubic L_4 term nevertheless makes the free energy $\mathcal{E}[Q]$ unbounded from below (Ball & Majumdar, 2010).

To address this issue, a Maier-Saupe type singular bulk potential ψ_B originally introduced in Katriel et al. (1986), was adopted in Ball and Majumdar (2010) to replace the regular potential $\mathcal{F}_{bulk}$. Specifically, the potential f is defined by

$$f(Q) \stackrel{\text{def}}{=} \begin{cases} \inf\limits_{\rho\in\mathcal{A}_Q} \displaystyle\int_{\mathbb{S}^2} \rho(\mathbf{n})\ln\rho(\mathbf{n})\,\mathrm{d}S, & -\dfrac{1}{3} < \lambda_i(Q) < \dfrac{2}{3},\ 1 \le i \le 3 \\ +\infty, & \text{otherwise,} \end{cases} \tag{1.6}$$

where the admissible set $\mathcal{A}_Q$ is

$$\mathcal{A}_Q = \left\{ \rho \in \mathcal{P}(\mathbb{S}^2) \middle| \rho(\mathbf{n}) = \rho(-\mathbf{n}), \int_{\mathbb{S}^2} \left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbb{I}_3\right)\rho(\mathbf{n})\,\mathrm{d}S = Q \right\}. \tag{1.7}$$

In other words, we minimize the Boltzmann entropy over all probability density functions ρ

with a given normalized second moment Q. Correspondingly,

$$\psi_{MS}(Q) = f(Q) - \frac{\kappa}{2}|Q|^2, \qquad \kappa > 0 \tag{1.8}$$

is used to replace the bulk potential $\mathcal{F}_{bulk}$. Note that the very last term is added to ensure the existence of multiple local energy minimizers. In this way, ψ_{MS} imposes a natural enforcement of a physical constraint on the eigenvalues of the mathematical Q-tensor, and henceforth the elastic energy part $\mathcal{F}_{el}$ is bounded from below. We refer interested readers to Xu (2022) and Zarnescu (2021) for a comprehensive list of the existing literature on the analytic study of this singular potential.

On the other hand, the regular bulk part $\mathcal{F}_{bulk}$ in the free energy (1.4) is typically a truncated expansion in the scalar invariants of the tensor Q (Paicu & Zarnescu, 2011, 2012)

$$\mathcal{F}_{bulk} = \frac{a}{2}\operatorname{tr}(Q^2) - \frac{b}{3}\operatorname{tr}(Q^3) + \frac{c}{4}\operatorname{tr}^2(Q^2), \tag{1.9}$$

where in the simplest case a, b, c are assumed to be material-dependent constants. Therefore, it is of natural interest to ask what values of a, b, c match with the asymptotic expansion of the singular potential $\psi_B(Q)$ (Ball, 2012) up to the 4-th order, which is the aim of this paper.

The main result of the paper is stated as follows.

Theorem 1.1. *As $Q \to 0$, the Maier-Saupe type bulk potential ψ_{MS} has the expansion*

$$\psi_{MS}(Q) = -\ln(4\pi) + \left(\frac{15}{4} - \frac{\kappa}{2}\right)\operatorname{tr}(Q^2) - \frac{75}{14}\operatorname{tr}(Q^3) + \frac{3825}{392}\operatorname{tr}(Q^4) + \cdots \tag{1.10}$$

The rest of the paper is organized as follows. In Section 2, we provide some prelimaries and the main idea on how to prove the main result Theorem 1.1. In Section 3, we perform all detailed derivations to complete its proof.

2 Preliminaries and strategy of the proof

As proved in Feireisl et al. (2014), f is smooth in the domain of the Q-tensor space where Q satisfies (1.2). Since f is rotation invariant, here and after, we always assume that any considered physical Q-tensor is diagonal:

$$Q = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}, \qquad -\frac{1}{3} < \lambda_1 \le \lambda_2 \le \lambda_3 < \frac{2}{3},\ \lambda_1+\lambda_2+\lambda_3 = 0. \tag{2.1}$$

Correspondingly the optimal density function $\rho^* \in \mathcal{A}_Q$ that satisfies $f(Q) = \int_{\mathbb{S}^2} \rho^* \ln \rho^* \,\mathrm{d}S$ is given by (Schimming et al., 2021)

$$\rho^*(x,y,z) = \frac{\exp(\mu_1 x^2 + \mu_2 y^2 + \mu_3 z^2)}{Z(\mu_1,\mu_2,\mu_3)}, \quad (x,y,z) \in \mathbb{S}^2, \quad \mu_1+\mu_2+\mu_3 = 0. \tag{2.2}$$

Here in (2.7), $Z(\mu_1,\mu_2,\mu_3)$ is given by

$$Z(\mu_1,\mu_2,\mu_3) = \int_{\mathbb{S}^2} \exp(\mu_1 x^2 + \mu_2 y^2 + \mu_3 z^2)\,\mathrm{d}S, \tag{2.3}$$

which satisfies

$$\frac{1}{Z}\frac{\partial Z}{\partial \mu_i} = \lambda_i + \frac{1}{3}, \qquad 1 \le i \le 3. \tag{2.4}$$

The first key ingredient in the proof of Theorem 1.1 is as follows. As the Q-tensor gets sufficiently close to 0, it can be represented by

$$Q_{\varepsilon,\eta} = \begin{pmatrix} \varepsilon & 0 & 0 \\ 0 & \eta & 0 \\ 0 & 0 & -(\varepsilon+\eta) \end{pmatrix}, \qquad |\varepsilon|, |\eta| \ll 1. \tag{2.5}$$

Thus the asymptotic expansion of f near $Q = 0$ is reformulated as the Taylor's expansion of the multi-variable smooth function $f(Q_{\varepsilon,\eta})$ that depends on ε, η. We shall compute the Taylor's expansion of $f(Q_{\varepsilon,\eta})$ at $\varepsilon = \eta = 0$ up to the 4-th order.

Meanwhile, we denote $\rho^*_{\varepsilon,\eta} \in \mathcal{A}_{Q_{\varepsilon,\eta}}$ the optimal density function that satisfies

$$f(Q_{\varepsilon,\eta}) = \int_{\mathbb{S}^2} \rho^*_{\varepsilon,\eta} \ln \rho^*_{\varepsilon,\eta} \mathrm{d}S, \tag{2.6}$$

which is given by

$$\rho^*_{\varepsilon,\eta}(x,y,z) = \frac{\exp(\mu_{1\varepsilon,\eta}x^2 + \mu_{2\varepsilon,\eta}y^2 + \mu_{3\varepsilon,\eta}z^2)}{Z(\mu_{1\varepsilon,\eta}, \mu_{2\varepsilon,\eta}, \mu_{3\varepsilon,\eta})}, \quad (x,y,z) \in \mathbb{S}^2, \tag{2.7}$$

$$\mu_{1\varepsilon,\eta} + \mu_{2\varepsilon,\eta} + \mu_{3\varepsilon,\eta} = 0. \tag{2.8}$$

Here Z is given by

$$Z(\mu_{1\varepsilon,\eta}, \mu_{2\varepsilon,\eta}, \mu_{3\varepsilon,\eta}) = \int_{\mathbb{S}^2} \exp(\mu_{1\varepsilon,\eta}x^2 + \mu_{2\varepsilon,\eta}y^2 + \mu_{3\varepsilon,\eta}z^2)\, \mathrm{d}S, \tag{2.9}$$

which satisfies

$$\frac{1}{Z}\frac{\partial Z}{\partial \mu_1} = \int_{\mathbb{S}^2} x^2 \rho^*_{\varepsilon,\eta}(x,y,z)\, \mathrm{d}S = \varepsilon + \frac{1}{3}, \tag{2.10}$$

$$\frac{1}{Z}\frac{\partial Z}{\partial \mu_2} = \int_{\mathbb{S}^2} y^2 \rho^*_{\varepsilon,\eta}(x,y,z)\, \mathrm{d}S = \eta + \frac{1}{3}, \tag{2.11}$$

$$\frac{1}{Z}\frac{\partial Z}{\partial \mu_3} = \int_{\mathbb{S}^2} z^2 \rho^*_{\varepsilon,\eta}(x,y,z)\, \mathrm{d}S = -(\varepsilon + \eta) + \frac{1}{3}. \tag{2.12}$$

The second key ingredient in the proof of Theorem 1.1 is the following reformulation of f. By virtue of (2.6)-(2.11), we see that

$$f(Q_{\varepsilon,\eta}) = \mu_{1\varepsilon,\eta}(2\varepsilon + \eta) + \mu_{2\varepsilon,\eta}(\varepsilon + 2\eta) - \ln Z(\mu_{1\varepsilon,\eta}, \mu_{2\varepsilon,\eta}, \mu_{3\varepsilon,\eta}). \tag{2.13}$$

Hence computation of derivatives of the function f depends on the computation of derivatives of the Lagrange multiplier functions $\mu_{1\varepsilon,\eta}, \mu_{2\varepsilon,\eta}$, as well as the renormalization function Z. Here and after, unless pointing out explicitly, we abbreviate $\mu_{1\varepsilon,\eta}, \mu_{2\varepsilon,\eta}$ by μ_1, μ_2, respectively.

The third key ingredient in the proof of Theorem 1.1 relies on the following derivations. We infer from (2.7)-(2.11) that

$$
\begin{aligned}
\frac{\partial \ln Z}{\partial \varepsilon} &= \frac{1}{Z}\frac{\partial Z}{\partial \varepsilon} = \frac{\partial \mu_1}{\partial \varepsilon}\int_{\mathbb{S}^2} \rho^*_{\varepsilon,\eta}(x^2 - z^2)\,\mathrm{d}S + \frac{\partial \mu_2}{\partial \varepsilon}\int_{\mathbb{S}^2} \rho^*_{\varepsilon,\eta}(y^2 - z^2)\,\mathrm{d}S \\
&= \frac{\partial \mu_1}{\partial \varepsilon}(2\varepsilon + \eta) + \frac{\partial \mu_2}{\partial \varepsilon}(\varepsilon + 2\eta), \qquad (2.14)\\
\frac{\partial \ln Z}{\partial \eta} &= \frac{1}{Z}\frac{\partial Z}{\partial \eta} = \frac{\partial \mu_1}{\partial \eta}\int_{\mathbb{S}^2} \rho^*_{\varepsilon,\eta}(x^2 - z^2)\,\mathrm{d}S + \frac{\partial \mu_2}{\partial \eta}\int_{\mathbb{S}^2} \rho^*_{\varepsilon,\eta}(y^2 - z^2)\,\mathrm{d}S \\
&= \frac{\partial \mu_1}{\partial \eta}(2\varepsilon + \eta) + \frac{\partial \mu_2}{\partial \eta}(\varepsilon + 2\eta), \qquad (2.15)
\end{aligned}
$$

which together with (2.13) implies

$$
\begin{aligned}
\frac{\partial f}{\partial \varepsilon} &= 2\mu_1 + \mu_2, \qquad (2.16)\\
\frac{\partial f}{\partial \eta} &= \mu_1 + 2\mu_2. \qquad (2.17)
\end{aligned}
$$

Therefore, it suffices to compute the derivatives of the Lagrange multiplier functions μ_1, μ_2 up to order 3.

3 Proof of the main result

In the next four subsections, we compute the 1-st to the 4-th order derivatives of f one by one. It is relatively straightforward to achieve lower order derivatives of f. However, to obtain the higher order derivatives of f, we need to make a full exploitation of equations (2.7)-(2.11).

3.1 Step 1: zero and first order derivatives of f

To begin with, at $Q = 0$ where $\varepsilon = \eta = 0$, it follows from Lu et al. (2022) that $\mu_1 = \mu_2 = \mu_3 = 0$. Hence $\rho^*_{0,0} = 1/4\pi$ and

$$
f(Q_{0,0}) = \int_{\mathbb{S}^2} \rho^*_{0,0} \ln \rho^*_{0,0}\,\mathrm{d}S = -\ln(4\pi). \qquad (3.1)
$$

And by (2.16) and (2.17) we see

$$\frac{\partial f}{\partial \varepsilon}\Big|_{\varepsilon=0} = \frac{\partial f}{\partial \eta}\Big|_{\eta=0} = 0. \tag{3.2}$$

3.2 Step 2: second order derivatives of f

Let us differentiate both sides of (2.10) and (2.11) w.r.t. ε. By (2.7), (2.14), and (2.15) we get

$$\Big[-\Big(\varepsilon+\frac{1}{3}\Big)(2\varepsilon+\eta)+\int_{\mathbb{S}^2} x^2(x^2-z^2)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S\Big]\frac{\partial \mu_1}{\partial \varepsilon} + \Big[-\Big(\varepsilon+\frac{1}{3}\Big)(\varepsilon+2\eta)+\int_{\mathbb{S}^2} x^2(y^2-z^2)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S\Big]\frac{\partial \mu_2}{\partial \varepsilon} = 1, \tag{3.3}$$

$$\Big[-\Big(\eta+\frac{1}{3}\Big)(2\varepsilon+\eta)+\int_{\mathbb{S}^2} y^2(x^2-z^2)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S\Big]\frac{\partial \mu_1}{\partial \varepsilon} + \Big[-\Big(\eta+\frac{1}{3}\Big)(\varepsilon+2\eta)+\int_{\mathbb{S}^2} y^2(y^2-z^2)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S\Big]\frac{\partial \mu_2}{\partial \varepsilon} = 0.. \tag{3.4}$$

Hence after we introduce the following functions (that depend on ε, η)

$$G_1 := -\Big(\varepsilon+\frac{1}{3}\Big)(2\varepsilon+\eta)+\int_{\mathbb{S}^2} x^2(x^2-z^2)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S, \tag{3.5}$$

$$G_2 := -\Big(\eta+\frac{1}{3}\Big)(\varepsilon+2\eta)+\int_{\mathbb{S}^2} y^2(y^2-z^2)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S, \tag{3.6}$$

$$G_3 := -\Big(\eta+\frac{1}{3}\Big)(2\varepsilon+\eta)+\int_{\mathbb{S}^2} y^2(x^2-z^2)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S, \tag{3.7}$$

$$G_4 := -\Big(\varepsilon+\frac{1}{3}\Big)(\varepsilon+2\eta)+\int_{\mathbb{S}^2} x^2(y^2-z^2)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S, \tag{3.8}$$

it yields from (3.3) and (3.4) that

$$\frac{\partial \mu_1}{\partial \varepsilon} = \frac{G_2}{G_1G_2-G_3G_4}, \tag{3.9}$$

$$\frac{\partial \mu_2}{\partial \varepsilon} = \frac{-G_3}{G_1G_2-G_3G_4}. \tag{3.10}$$

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Analogously, after differentiating equations (2.10) and (2.11) w.r.t. η, we obtain that

$$\frac{\partial \mu_1}{\partial \eta} = \frac{-G_4}{G_1G_2 - G_3G_4}, \tag{3.11}$$

$$\frac{\partial \mu_2}{\partial \eta} = \frac{G_1}{G_1G_2 - G_3G_4}. \tag{3.12}$$

Evaluating at $\varepsilon = \eta = 0$, we have $\rho^* = 1/4\pi$ and henceforth

$$G_1\Big|_{\varepsilon=\eta=0} = G_2\Big|_{\varepsilon=\eta=0} = \frac{2}{15}, \quad G_3\Big|_{\varepsilon=\eta=0} = G_4\Big|_{\varepsilon=\eta=0} = 0, \tag{3.13}$$

$$\frac{\partial \mu_1}{\partial \varepsilon}\Big|_{\varepsilon=\eta=0} = \frac{\partial \mu_2}{\partial \eta}\Big|_{\varepsilon=\eta=0} = \frac{15}{2}, \quad \frac{\partial \mu_1}{\partial \eta}\Big|_{\varepsilon=\eta=0} = \frac{\partial \mu_2}{\partial \varepsilon}\Big|_{\varepsilon=\eta=0} = 0. \tag{3.14}$$

Thus we conclude from (2.16)-(2.17) that

$$\frac{\partial^2 f}{\partial \varepsilon^2}\Big|_{\varepsilon=\eta=0} = \frac{\partial^2 f}{\partial \eta^2}\Big|_{\varepsilon=\eta=0} = 15, \quad \frac{\partial^2 f}{\partial \varepsilon \partial \eta}\Big|_{\varepsilon=\eta=0} = \frac{15}{2}. \tag{3.15}$$

In all, we collect all 2-nd order terms in the Taylor expansion and obtain

$$\frac{1}{2!}\left(\frac{\partial^2 f}{\partial \varepsilon^2}\Big|_{\varepsilon=\eta=0}\varepsilon^2 + 2\frac{\partial^2 f}{\partial \varepsilon \partial \eta}\Big|_{\varepsilon=\eta=0}\varepsilon\eta + \frac{\partial^2 f}{\partial \eta^2}\Big|_{\varepsilon=\eta=0}\eta^2\right) = \frac{15}{2}(\varepsilon^2 + \eta^2 + \varepsilon\eta) = \frac{15}{4}|Q_{\varepsilon,\eta}|^2. \tag{3.16}$$

3.3 Step 3: third order derivatives of f

By (2.7)-(2.8), $\rho^*_{\varepsilon,\eta}$ can be reformulated as

$$\rho^*_{\varepsilon,\eta} = \frac{\exp\left\{\mu_1(x^2 - z^2) + \mu_2(y^2 - z^2)\right\}}{Z}, \tag{3.17}$$

which together with (2.14) gives

$$\frac{\partial \rho^*_{\varepsilon,\eta}}{\partial \varepsilon} = \left[-(2\varepsilon + \eta)\frac{\partial \mu_1}{\partial \varepsilon} - (\varepsilon + 2\eta)\frac{\partial \mu_2}{\partial \varepsilon} + (x^2 - z^2)\frac{\partial \mu_1}{\partial \varepsilon} + (y^2 - z^2)\frac{\partial \mu_2}{\partial \varepsilon}\right]\rho^*_{\varepsilon,\eta}. \tag{3.18}$$

Thus we obtain from (3.5)-(3.8) and (2.14) that

$$\frac{\partial G_1}{\partial \varepsilon} = \frac{\partial \mu_1}{\partial \varepsilon} \int_{\mathbb{S}^2} x^2(x^2-z^2)(x^2-z^2-2\varepsilon-\eta)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S + \frac{\partial \mu_2}{\partial \varepsilon} \int_{\mathbb{S}^2} x^2(x^2-z^2)(y^2-z^2-\varepsilon-2\eta)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S - 4\varepsilon - \eta - \frac{2}{3}, \tag{3.19}$$

$$\frac{\partial G_2}{\partial \varepsilon} = \frac{\partial \mu_1}{\partial \varepsilon} \int_{\mathbb{S}^2} y^2(y^2-z^2)(x^2-z^2-2\varepsilon-\eta)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S + \frac{\partial \mu_2}{\partial \varepsilon} \int_{\mathbb{S}^2} y^2(y^2-z^2)(y^2-z^2-\varepsilon-2\eta)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S - \eta - \frac{1}{3}, \tag{3.20}$$

$$\frac{\partial G_3}{\partial \varepsilon} = \frac{\partial \mu_1}{\partial \varepsilon} \int_{\mathbb{S}^2} y^2(x^2-z^2)(x^2-z^2-2\varepsilon-\eta)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S + \frac{\partial \mu_2}{\partial \varepsilon} \int_{\mathbb{S}^2} y^2(x^2-z^2)(y^2-z^2-\varepsilon-2\eta)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S - 2\eta - \frac{2}{3}, \tag{3.21}$$

$$\frac{\partial G_4}{\partial \varepsilon} = \frac{\partial \mu_1}{\partial \varepsilon} \int_{\mathbb{S}^2} x^2(y^2-z^2)(x^2-z^2-2\varepsilon-\eta)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S + \frac{\partial \mu_2}{\partial \varepsilon} \int_{\mathbb{S}^2} x^2(y^2-z^2)(y^2-z^2-\varepsilon-2\eta)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S - 2\varepsilon - 2\eta - \frac{1}{3}. \tag{3.22}$$

Evaluating at $\varepsilon = \eta = 0$, we see $\rho^*_{0,0} = 1/4\pi$ and by (3.14) we have

$$\left.\frac{\partial G_1}{\partial \varepsilon}\right|_{\varepsilon=\eta=0} = \frac{15}{8\pi} \int_{\mathbb{S}^2} x^2(x^2-z^2)^2\,\mathrm{d}S - \frac{2}{3} = \frac{4}{21}, \tag{3.23}$$

$$\left.\frac{\partial G_2}{\partial \varepsilon}\right|_{\varepsilon=\eta=0} = \frac{15}{8\pi} \int_{\mathbb{S}^2} y^2(y^2-z^2)(x^2-z^2)\,\mathrm{d}S - \frac{1}{3} = -\frac{4}{21}, \tag{3.24}$$

$$\left.\frac{\partial G_3}{\partial \varepsilon}\right|_{\varepsilon=\eta=0} = \frac{15}{8\pi} \int_{\mathbb{S}^2} y^2(x^2-z^2)^2\,\mathrm{d}S - \frac{2}{3} = -\frac{8}{21}, \tag{3.25}$$

$$\left.\frac{\partial G_4}{\partial \varepsilon}\right|_{\varepsilon=\eta=0} = \frac{15}{8\pi} \int_{\mathbb{S}^2} x^2(x^2-z^2)(y^2-z^2)\,\mathrm{d}S - \frac{1}{3} = -\frac{4}{21}. \tag{3.26}$$

As a consequence, together with (3.9), (3.10) and (3.13) we conclude that

$$\left.\frac{\partial^2 \mu_1}{\partial \varepsilon^2}\right|_{\varepsilon=\eta=0} = \left.\frac{-\frac{\partial G_1}{\partial \varepsilon}}{G_1^2}\right|_{\varepsilon=\eta=0} = -\frac{75}{7}, \tag{3.27}$$

$$\left.\frac{\partial^2 \mu_2}{\partial \varepsilon^2}\right|_{\varepsilon=\eta=0} = \left.\frac{-\frac{\partial G_3}{\partial \varepsilon}}{G_1 G_2}\right|_{\varepsilon=\eta=0} = \frac{150}{7}. \tag{3.28}$$

Thus we infer from (2.16) that

$$\frac{\partial^3 f}{\partial \varepsilon^3}\bigg|_{\varepsilon=\eta=0} = 2\frac{\partial^2 \mu_1}{\partial \varepsilon^2}\bigg|_{\varepsilon=\eta=0} + \frac{\partial^2 \mu_2}{\partial \varepsilon^2}\bigg|_{\varepsilon=\eta=0} = 0. \tag{3.29}$$

At the same time, we infer from (2.15) that

$$\frac{\partial \rho^*_{\varepsilon,\eta}}{\partial \eta} = \Big[-(2\varepsilon+\eta)\frac{\partial \mu_1}{\partial \eta} - (\varepsilon+2\eta)\frac{\partial \mu_2}{\partial \eta} + (x^2-z^2)\frac{\partial \mu_1}{\partial \eta} + (y^2-z^2)\frac{\partial \mu_2}{\partial \eta}\Big]\rho^*_{\varepsilon,\eta}. \tag{3.30}$$

Together with (3.5)-(3.8), we obtain

$$\begin{aligned}
\frac{\partial G_1}{\partial \eta} &= \frac{\partial \mu_1}{\partial \eta}\int_{\mathbb{S}^2} x^2(x^2-z^2)(x^2-z^2-2\varepsilon-\eta)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S \\
&\quad + \frac{\partial \mu_2}{\partial \eta}\int_{\mathbb{S}^2} x^2(x^2-z^2)(y^2-z^2-\varepsilon-2\eta)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S - \varepsilon - \frac{1}{3}, &(3.31)\\
\frac{\partial G_2}{\partial \eta} &= \frac{\partial \mu_1}{\partial \eta}\int_{\mathbb{S}^2} y^2(y^2-z^2)(x^2-z^2-2\varepsilon-\eta)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S \\
&\quad + \frac{\partial \mu_2}{\partial \eta}\int_{\mathbb{S}^2} y^2(y^2-z^2)(y^2-z^2-\varepsilon-2\eta)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S - \varepsilon - 4\eta - \frac{2}{3}, &(3.32)\\
\frac{\partial G_3}{\partial \eta} &= \frac{\partial \mu_1}{\partial \eta}\int_{\mathbb{S}^2} y^2(x^2-z^2)(x^2-z^2-2\varepsilon-\eta)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S \\
&\quad + \frac{\partial \mu_2}{\partial \eta}\int_{\mathbb{S}^2} y^2(x^2-z^2)(y^2-z^2-\varepsilon-2\eta)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S - 2\varepsilon - 2\eta - \frac{1}{3}, &(3.33)\\
\frac{\partial G_4}{\partial \eta} &= \frac{\partial \mu_1}{\partial \eta}\int_{\mathbb{S}^2} x^2(y^2-z^2)(x^2-z^2-2\varepsilon-\eta)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S \\
&\quad + \frac{\partial \mu_2}{\partial \eta}\int_{\mathbb{S}^2} x^2(y^2-z^2)(y^2-z^2-\varepsilon-2\eta)\rho^*_{\varepsilon,\eta}\,\mathrm{d}S - 2\varepsilon - \frac{2}{3}. &(3.34)
\end{aligned}$$

Evaluating at $\varepsilon=\eta=0$, then $\rho^*_{0,0} = 1/4\pi$ and (3.14) implies

$$\begin{aligned}
\frac{\partial G_1}{\partial \eta}\bigg|_{\varepsilon=\eta=0} &= \frac{15}{8\pi}\int_{\mathbb{S}^2} x^2(x^2-z^2)(y^2-z^2)\,\mathrm{d}S - \frac{1}{3} = -\frac{4}{21}, &(3.35)\\
\frac{\partial G_2}{\partial \eta}\bigg|_{\varepsilon=\eta=0} &= \frac{15}{8\pi}\int_{\mathbb{S}^2} y^2(y^2-z^2)^2\,\mathrm{d}S - \frac{2}{3} = \frac{4}{21}, &(3.36)\\
\frac{\partial G_3}{\partial \eta}\bigg|_{\varepsilon=\eta=0} &= \frac{15}{8\pi}\int_{\mathbb{S}^2} y^2(x^2-z^2)(y^2-z^2)\,\mathrm{d}S - \frac{1}{3} = -\frac{4}{21}, &(3.37)
\end{aligned}$$

$$\frac{\partial G_4}{\partial \eta}\bigg|_{\varepsilon=\eta=0} = \frac{15}{8\pi}\int_{\mathbb{S}^2} x^2(y^2-z^2)^2\,\mathrm{d}S - \frac{1}{3} = -\frac{8}{21}. \tag{3.38}$$

As a consequence, we get from (3.9)-(3.13) that

$$\frac{\partial^2 \mu_1}{\partial \eta^2}\bigg|_{\varepsilon=\eta=0} = \frac{-\frac{\partial G_4}{\partial \eta}}{G_1 G_2}\bigg|_{\varepsilon=\eta=0} = \frac{150}{7}, \tag{3.39}$$

$$\frac{\partial^2 \mu_2}{\partial \eta^2}\bigg|_{\varepsilon=\eta=0} = \frac{-\frac{\partial G_2}{\partial \eta}}{G_2^2}\bigg|_{\varepsilon=\eta=0} = -\frac{75}{7}, \tag{3.40}$$

$$\frac{\partial^2 \mu_1}{\partial \varepsilon \partial \eta}\bigg|_{\varepsilon=\eta=0} = \frac{-\frac{\partial G_1}{\partial \eta}}{G_1^2}\bigg|_{\varepsilon=\eta=0} = \frac{75}{7}, \tag{3.41}$$

$$\frac{\partial^2 \mu_2}{\partial \varepsilon \partial \eta}\bigg|_{\varepsilon=\eta=0} = \frac{-\frac{\partial G_3}{\partial \eta}}{G_1 G_2}\bigg|_{\varepsilon=\eta=0} = \frac{75}{7} \tag{3.42}$$

Therefore we infer from (2.16)-(2.17) that

$$\frac{\partial^3 f}{\partial \eta^3}\bigg|_{\varepsilon=\eta=0} = \frac{\partial^2 \mu_1}{\partial \eta^2}\bigg|_{\varepsilon=\eta=0} + 2\frac{\partial^2 \mu_2}{\partial \eta^2}\bigg|_{\varepsilon=\eta=0} = 0, \tag{3.43}$$

$$\frac{\partial^3 f}{\partial \varepsilon \partial \eta^2}\bigg|_{\varepsilon=\eta=0} = \frac{\partial^2 \mu_1}{\partial \varepsilon \partial \eta}\bigg|_{\varepsilon=\eta=0} + 2\frac{\partial^2 \mu_2}{\partial \varepsilon \partial \eta}\bigg|_{\varepsilon=\eta=0} = \frac{225}{7}, \tag{3.44}$$

$$\frac{\partial^3 f}{\partial \varepsilon^2 \partial \eta}\bigg|_{\varepsilon=\eta=0} = 2\frac{\partial^2 \mu_1}{\partial \varepsilon \partial \eta}\bigg|_{\varepsilon=\eta=0} + \frac{\partial^2 \mu_2}{\partial \varepsilon \partial \eta}\bigg|_{\varepsilon=\eta=0} = \frac{225}{7}. \tag{3.45}$$

To sum up, all the 3-rd order terms (3.29), (3.43)-(3.45) in the Taylor's expansion together contribute to

$$\begin{aligned} &\frac{1}{3!}\Big(\frac{\partial^3 f}{\partial \varepsilon^3}\bigg|_{\varepsilon=\eta=0}\varepsilon^3 + 3\frac{\partial^3 f}{\partial \varepsilon \partial \eta^2}\bigg|_{\varepsilon=\eta=0}\varepsilon\eta^2 + 3\frac{\partial^3 f}{\partial \varepsilon^2 \partial \eta}\bigg|_{\varepsilon=\eta=0}\varepsilon^2\eta + \frac{\partial^3 f}{\partial \eta^3}\bigg|_{\varepsilon=\eta=0}\eta^3\Big) \\ &= \frac{75}{14}(3\varepsilon^2\eta + 3\varepsilon\eta^2) = \frac{75}{14}\big[-\varepsilon^3 - \eta^3 + (\varepsilon+\eta)^3\big] = \frac{75}{14}\,\mathrm{tr}\left(Q^3_{\varepsilon,\eta}\right). \end{aligned} \tag{3.46}$$

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3.4 Step 4: fourth order derivatives of f

By (2.16)-(2.17) and (3.9)-(3.12), it suffices to compute the second order derivatives of $G_1, \cdots, G_4$ w.r.t. ε, η. To begin with, it follows from (3.19) that

$$\begin{aligned}\frac{\partial^2 G_1}{\partial \varepsilon^2} = -4 - \Big[2\frac{\partial \mu_1}{\partial \varepsilon} + \frac{\partial \mu_2}{\partial \varepsilon} + (2\varepsilon+\eta)\frac{\partial^2 \mu_1}{\partial \varepsilon^2} + (\varepsilon+2\eta)\frac{\partial^2 \mu_2}{\partial \varepsilon^2}\Big]\int_{\mathbb{S}^2} x^2(x^2-z^2)\rho^* \\ - \Big[(2\varepsilon+\eta)\frac{\partial \mu_1}{\partial \varepsilon} + (\varepsilon+2\eta)\frac{\partial \mu_2}{\partial \varepsilon}\Big]\int_{\mathbb{S}^2} x^2(x^2-z^2)\frac{\partial \rho^*}{\partial \varepsilon} + \frac{\partial^2 \mu_1}{\partial \varepsilon^2}\int_{\mathbb{S}^2} x^2(x^2-z^2)^2\rho^* \\ + \frac{\partial \mu_1}{\partial \varepsilon}\int_{\mathbb{S}^2} x^2(x^2-z^2)^2\frac{\partial \rho^*}{\partial \varepsilon} + \frac{\partial^2 \mu_2}{\partial \varepsilon^2}\int_{\mathbb{S}^2} x^2(x^2-z^2)(y^2-z^2)\rho^* \\ + \frac{\partial \mu_2}{\partial \varepsilon}\int_{\mathbb{S}^2} x^2(x^2-z^2)(y^2-z^2)\frac{\partial \rho^*}{\partial \varepsilon}. \end{aligned} \tag{3.47}$$

Since (3.14) gives $\frac{\partial \mu_2}{\partial \varepsilon}\Big|_{\varepsilon=\eta=0} = 0$, together with (3.18) we see that the evaluation of (3.47) at $\varepsilon = \eta = 0$ is reduced to

$$\begin{aligned}\frac{\partial^2 G_1}{\partial \varepsilon^2}\Big|_{\varepsilon=\eta=0} = \Big\{ -4 - 2\frac{\partial \mu_1}{\partial \varepsilon}\int_{\mathbb{S}^2} x^2(x^2-z^2)\rho^* + \frac{\partial^2 \mu_1}{\partial \varepsilon^2}\int_{\mathbb{S}^2} x^2(x^2-z^2)^2\rho^* \\ + \Big(\frac{\partial \mu_1}{\partial \varepsilon}\Big)^2\int_{\mathbb{S}^2} x^2(x^2-z^2)^3\rho^* + \frac{\partial^2 \mu_2}{\partial \varepsilon^2}\int_{\mathbb{S}^2} x^2(x^2-z^2)(y^2-z^2)\rho^* \Big\}\Big|_{\varepsilon=\eta=0} \end{aligned} \tag{3.48}$$

Evaluating (3.48) at $\varepsilon = \eta = 0$, together with (3.14), (3.27), (3.28) we have

$$\begin{aligned}\frac{\partial^2 G_1}{\partial \varepsilon^2}\Big|_{\varepsilon=\eta=0} &= -4 - \frac{15}{4\pi}\int_{\mathbb{S}^2} x^2(x^2-z^2) - \frac{75}{28\pi}\int_{\mathbb{S}^2} x^2(x^2-z^2)^2 \\ &\quad + \frac{225}{16\pi}\int_{\mathbb{S}^2} x^2(x^2-z^2)^3 + \frac{75}{14\pi}\int_{\mathbb{S}^2} x^2(x^2-z^2)(y^2-z^2) \\ &= -4 - \frac{15}{4\pi}\frac{8\pi}{15} - \frac{75}{28\pi}\frac{16\pi}{35} + \frac{225}{16\pi}\frac{32\pi}{105} + \frac{75}{14\pi}\frac{8\pi}{105} \\ &= -\frac{124}{49} \end{aligned} \tag{3.49}$$

Similarly, we find

$$\frac{\partial^2 G_2}{\partial \varepsilon^2}\Big|_{\varepsilon=\eta=0} = \frac{12}{49}, \quad \frac{\partial^2 G_3}{\partial \varepsilon^2}\Big|_{\varepsilon=\eta=0} = 0, \quad \frac{\partial^2 G_4}{\partial \varepsilon^2}\Big|_{\varepsilon=\eta=0} = -\frac{68}{49}. \tag{3.50}$$

Next, for the sake of convenience, we introduce the function (that depends on ε, η)

$$F = G_1 G_2 - G_3 G_4. \tag{3.51}$$

Then it is ready to check from (3.13), (3.35)-(3.38), (3.49)-(3.50) that

$$F\Big|_{\varepsilon=\eta=0} = \frac{4}{225}, \quad \frac{\partial F}{\partial \varepsilon}\Big|_{\varepsilon=\eta=0} = 0, \quad \frac{\partial^2 F}{\partial \varepsilon^2}\Big|_{\varepsilon=\eta=0} = -\frac{128}{245} \tag{3.52}$$

As consequence, together with (3.9)-(3.10), (3.13), and (3.49)-(3.50) we have

$$\frac{\partial^3 \mu_1}{\partial \varepsilon^3}\Big|_{\varepsilon=\eta=0} = \frac{1}{F^2}\Big(\frac{\partial^2 G_2}{\partial \varepsilon^2} F - G_2 \frac{\partial^2 F}{\partial \varepsilon^2}\Big)\Big|_{\varepsilon=\eta=0} - \frac{2}{F^3}\frac{\partial F}{\partial \varepsilon}\Big(\frac{\partial G_2}{\partial \varepsilon} F - G_2 \frac{\partial F}{\partial \varepsilon}\Big)\Big|_{\varepsilon=\eta=0} = \frac{11475}{49}, \tag{3.53}$$

$$\frac{\partial^3 \mu_2}{\partial \varepsilon^3}\Big|_{\varepsilon=\eta=0} = -\frac{1}{F^2}\Big(\frac{\partial^2 G_3}{\partial \varepsilon^2} F - G_3 \frac{\partial^2 F}{\partial \varepsilon^2}\Big)\Big|_{\varepsilon=\eta=0} + \frac{2}{F^3}\frac{\partial F}{\partial \varepsilon}\Big(\frac{\partial G_3}{\partial \varepsilon} F - G_3 \frac{\partial F}{\partial \varepsilon}\Big)\Big|_{\varepsilon=\eta=0} = 0. \tag{3.54}$$

Analogously, we get

$$\frac{\partial^3 \mu_1}{\partial \eta^3}\Big|_{\varepsilon=\eta=0} = 0, \quad \frac{\partial^3 \mu_2}{\partial \eta^3}\Big|_{\varepsilon=\eta=0} = \frac{11475}{49}, \tag{3.55}$$

$$\frac{\partial^3 \mu_1}{\partial \eta \partial \varepsilon^2}\Big|_{\varepsilon=\eta=0} = \frac{\partial^3 \mu_1}{\partial \varepsilon \partial \eta^2}\Big|_{\varepsilon=\eta=0} = \frac{\partial^3 \mu_2}{\partial \eta \partial \varepsilon^2}\Big|_{\varepsilon=\eta=0} = \frac{\partial^3 \mu_2}{\partial \varepsilon \partial \eta^2}\Big|_{\varepsilon=\eta=0} = \frac{3825}{49}. \tag{3.56}$$

Thus in view of (2.16), (2.17), and (3.53)-(3.56), we obtain

$$\frac{\partial^4 f}{\partial \varepsilon^4}\Big|_{\varepsilon=\eta=0} = \frac{\partial^4 f}{\partial \eta^4}\Big|_{\varepsilon=\eta=0} = \frac{22950}{49}, \tag{3.57}$$

$$\frac{\partial^4 f}{\partial \varepsilon \partial \eta^3}\Big|_{\varepsilon=\eta=0} = \frac{\partial^4 f}{\partial \varepsilon^2 \partial \eta^2}\Big|_{\varepsilon=\eta=0} = \frac{\partial^4 f}{\partial \eta \partial \varepsilon^3}\Big|_{\varepsilon=\eta=0} = \frac{11475}{49}. \tag{3.58}$$

In all, we collect all 4-th order terms in (3.57)-(3.58) in the Taylor expansion and obtain

$$\frac{1}{4!}\Big(\frac{\partial^4 f}{\partial \varepsilon^4}\Big|_{\varepsilon=\eta=0}\varepsilon^4 + 4\frac{\partial^4 f}{\partial \varepsilon \partial \eta^3}\Big|_{\varepsilon=\eta=0}\varepsilon\eta^3 + 6\frac{\partial^4 f}{\partial \varepsilon^2 \partial \eta^2}\Big|_{\varepsilon=\eta=0}\varepsilon^2\eta^2 + 4\frac{\partial^4 f}{\partial \eta \partial \varepsilon^3}\Big|_{\varepsilon=\eta=0}\eta\varepsilon^3 + \frac{\partial^4 f}{\partial \eta^4}\Big|_{\varepsilon=\eta=0}\eta^4\Big)$$

$$= \frac{3825}{392}(2\varepsilon^4 + 4\varepsilon\eta^3 + 6\varepsilon^2\eta^2 + 4\varepsilon^3\eta + 2\eta^4) = \frac{3825}{392}\left[\varepsilon^4 + \eta^4 + (\varepsilon + \eta)^4\right] = \frac{3825}{392}\,\mathrm{tr}\left(Q^4_{\varepsilon,\eta}\right). \tag{3.59}$$

Therefore, the proof of Theorem 1.1 is complete after we put together (3.1), (3.2), (3.16), (3.46), and (3.59).

Remark 3.1. *A prediction regarding the asymptotic expansion of the very singular potential near the nematic-transition point is given in Ball (2012), which reads*

$$\psi_{MS}(Q) = -\ln(4\pi) + \left(\frac{15}{4} - \frac{\kappa}{2}\right)\mathrm{tr}(Q^2) - \frac{75}{14}\mathrm{tr}(Q^3) + \frac{225}{112}\mathrm{tr}(Q^4) + \cdots \tag{3.60}$$

which is consistent with Theorem 1.1 up to the 3rd order.

4 Conclusion

We focus on a singular bulk potential within the framework of Q-tensor theory for modeling nematic liquid crystals. This theory provides a thermodynamically consistent framework that accurately describes free energy and phase transitions, and it is essential for practical applications such as optimizing liquid crystal displays and sensors. Additionally, it offers a rich mathematical structure for studying partial differential equations and multi-physics interactions. The main purpose of this paper is to calculate the asymptotic expansion of this potential near the nematic-isotropic transition point up to the 4-th order, which helps identify universal behavior in phase transition and contributes to broader theoretical frameworks in statistical mechanics. The refined expansion also opens avenues for extending this framework to other types of phase transitions in complex systems. Asymptotic expansions can provide manageable approximations that reveal leading-order behaviors in specific limits. This study enhances our understanding of system behavior near critical points and guides the development of numerical methods, further optimizing the performance of liquid crystal-based material with tailored transition behavior.

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