Journal of Nonlinear Science (2022) 32:6
https://doi.org/10.1007/s00332-021-09761-x

Blowup Rate Estimates of a Singular Potential and Its Gradient in the Landau-de Gennes Theory

Xin Yang Lu[1,2] · Xiang Xu[3] · Wujun Zhang[4]

Received: 29 April 2021 / Accepted: 13 October 2021 / Published online: 4 November 2021

Abstract

In this paper, we revisit a singular bulk potential in the Landau-de Gennes free energy that describes nematic liquid crystal configurations in the framework of the Q-tensor order parameter. This Maier–Saupe type singular potential was originally introduced in Katriel et al. (Mol Cryst Liquid Cryst 1:337–355, 1986), which is considered as a natural enforcement of a physical constraint on the eigenvalues of symmetric, traceless Q-tensors. Specifically, we establish blowup rates of both this singular potential and its gradient as Q approaches its physical boundary. All of the proofs are elementary.

Keywords Liquid crystals · Q-tensor · Singular potential · Blowup rate

MSC codes 35B44 · 35Q82

1 Introduction

Liquid crystals are an intermediate state of matter between the commonly observed solid and liquid that has no or partial positional order but do exhibit an orientation

Dedicated to Professor David Kinderlehrer's 80th birthday.

Communicated by Eliot Fried.

✉ Xiang Xu
x2xu@odu.edu

Xin Yang Lu
xlu8@lakeheadu.ca

Wujun Zhang
wujun@math.rutgers.edu

1 Department of Mathematical Sciences, Lakehead University, Thunder Bay, Canada

2 Department of Mathematics and Statistics, McGill University, Montréal, Canada

3 Department of Mathematics and Statistics, Old Dominion University, Norfolk, VA 23529, USA

4 Department of Mathematics, Rutgers University, New Brunswick, NJ 08901, USA

order, and the simplest form of liquid crystals is called nematic type. Broadly speaking, there are two types of models to describe nematic liquid crystals, namely the mean field model and the continuum model. In the former one, the local alignment of liquid crystal molecules is described by a probability distribution function on the unit sphere (de Gennes and Prost 1993; Maier and Saupe 1959; Virga 1994). Let $\mathbf{n}$ be a unit vector in $\mathbb{R}^3$, representing the orientation of a single liquid crystal molecule, and $\rho(x;\mathbf{n})$ be the density distribution function of the orientation of all molecules at a point $x \in \Omega \subset \mathbb{R}^3$. The de Gennes Q-tensor, defined as the deviation of the second moment of ρ from its isotropic value, reads

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

Note that de Gennes Q-tensor vanishes in the isotropic phase, and hence it serves as an order parameter. Meanwhile, it follows immediately from (1.1) that any de Gennes Q-tensor is symmetric, traceless, and all its eigenvalues satisfy the constraint $-1/3 \le \lambda_i(Q) \le 2/3$, $1 \le i \le 3$.

In the continuum model, instead, a phenomenological Landau-de Gennes theory is proposed (Ball 2012; de Gennes and Prost 1993; Mottram and Newton 2014) such that the alignment of liquid crystal molecules is described by the macroscopic Q-tensor order parameter, which is a symmetric, traceless 3×3 matrix without any eigenvalue constraint. In contrast with the de Gennes Q-tensor in the mean field model, this microscopic order parameter in the Landau-de Gennes theory is at times referred to as the mathematical Q-tensor. In this framework the free energy functional is derived as a nonlinear integral functional of the Q-tensor and its spatial derivatives (Ball 2012; Majumdar 2010):

$$\mathcal{E}[Q] = \int_{\Omega} \mathcal{F}(Q(x))\,\mathrm{d}x, \tag{1.2}$$

where Q is the basic element in the so-called Q-tensor space (Ball 2012)

$$\mathbb{Q} \overset{\text{def}}{=} \Big\{ M \in \mathbb{R}^{3\times3} \;\Big|\; \operatorname{tr}(M) = 0,\ M^T = M \Big\}. \tag{1.3}$$

The free energy density functional $\mathcal{F}$ is composed of the elastic part $\mathcal{F}_{el}$ that depends on the gradient of Q, as well as the bulk part $\mathcal{F}_{bulk}$ that depends on Q only. The bulk part $\mathcal{F}_{bulk}$ is typically a truncated expansion in the scalar invariants of the tensor Q (Majumdar and Zarnescu 2010; Paicu and Zarnescu 2011, 2012)

$$\mathcal{F}_{bulk} = \frac{a}{2}\operatorname{tr}(Q^2) - \frac{b}{3}\operatorname{tr}(Q^3) + \frac{c}{4}\operatorname{tr}^2(Q^2), \tag{1.4}$$

where a, b, c are assumed to be material-dependent coefficients. While the simplest form of the elastic part $\mathcal{F}_{el}$ that is invariant under rigid rotations and material symmetry is (Ball 2012; Ball and 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, $\partial_k Q_{ij}$ stands for 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. It is noted that the retention of the L_4 cubic term is that it allows complete reduction to the classical Oseen–Frank energy of liquid crystals with four elastic terms (Berreman and Meiboom 1984; Dickmann 1995; Iyer et al. 2015). On the other hand, however, this cubic term makes the free energy $\mathcal{E}[Q]$ unbounded from below (Ball and Majumdar 2010).

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

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

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 distributions ρ with given normalized second moment Q. Correspondingly,

$$\psi_B(Q) = f(Q) - \alpha |Q|^2 \tag{1.8}$$

is used to replace the commonly employed bulk potential $\mathcal{F}_{el}$. Note that the last polynomial term involves the intermolecular interaction kernel (Maier and Saupe 1959) and it represents anisotropic contribution to the energy per particle (Katriel et al. 1986). Further, it is added to ensure the existence of local energy minimizers, where $\alpha > 0$ is a constant. As a consequence, ψ_B imposes a natural enforcement of a physical constraint on the eigenvalues of the mathematical Q-tensor. Further, the elastic energy part $\mathcal{F}_{el}$ could be kept under control under mild assumptions on $L_1, \cdots L_4$ (Davis and Gartland 1998; Iyer et al. 2015; Kitavtsev et al. 2016). Interested readers may also see Golovaty et al. (2020a, b) where a new Landau-de Gennes model with quartic elastic energy terms is proposed.

Analysis of this singular potential is undoubtedly not straightforward, and there has been some development in recent years. Concerning dynamic configurations, in a non-isothermal co-rotational Beris–Edwards system whose free energy consists of one elastic constant term, namely L_1 term and this singular potential, the existence of global in time weak solutions is established in Feireisl et al. (2014, 2015), and the convexity of f is proved in Feireisl et al. (2015). The existence, regularity and strict physicality of global weak solutions of the corresponding isothermal co-rotational Beris–Edwards system in a $2D$ torus is investigated in Wilkinson (2015), while global existence and partial regularity of a suitable weak solution to this system in $3D$ is established in Du et al. (2020). The eigenvalue preservation of the co-rotational Beris–Edwards system with the regular bulk potential is studied in Wu et al. (2019) by virtue of f. On the other hand, in static configurations, the Hölder regularity of global energy minimizer in $2D$ is established in Bauman and Phillips (2016), while partial regularity results for the global energy minimizer are given in Evans et al. (2016), and further improved in Evans et al. (2016) under various assumptions of the blowup rates of f and its gradient as Q approaches its physical boundary. However, such assumptions are yet to be verified.

In static settings, the absolute minimizer of the free energy $\mathcal{E}$ satisfies the Euler–Lagrange equation

$$\begin{aligned} &2L_1\Delta Q_{ij} + (L_2+L_3)\Big(\partial_k\partial_j Q_{ik} + \partial_k\partial_i Q_{jk} - \frac{2}{3}\partial_k\partial_l Q_{kl}\delta_{ij}\Big) + 2L_4\partial_k(Q_{lk}\partial_l Q_{ij}) \\ &\quad - L_4\partial_i Q_{kl}\partial_j Q_{kl} + \frac{L_4|\nabla Q|^2}{3}\delta_{ij} - \frac{\partial f}{\partial Q_{ij}} + \frac{1}{3}\operatorname{tr}\Big(\frac{\partial f}{\partial Q}\Big)\delta_{ij} + 2\alpha Q_{ij} = 0, \qquad 1 \le i, j \le 3. \end{aligned} \tag{1.9}$$

While in dynamic settings, a solution to an L^2 gradient flow generated by $\mathcal{E}$ satisfies

$$\begin{aligned} \partial_t Q_{ij} &= 2L_1\Delta Q_{ij} + (L_2+L_3)\Big(\partial_k\partial_j Q_{ik} + \partial_k\partial_i Q_{jk} - \frac{2}{3}\partial_k\partial_l Q_{kl}\delta_{ij}\Big) + 2L_4\partial_k(Q_{lk}\partial_l Q_{ij}) \\ &\quad - L_4\partial_i Q_{kl}\partial_j Q_{kl} + \frac{L_4|\nabla Q|^2}{3}\delta_{ij} - \frac{\partial f}{\partial Q_{ij}} + \frac{1}{3}\operatorname{tr}\Big(\frac{\partial f}{\partial Q}\Big)\delta_{ij} + 2\alpha Q_{ij}, \qquad 1 \le i, j \le 3. \end{aligned} \tag{1.10}$$

If Q stays away from its physical boundary, then both f and $\partial f/\partial Q$ are bounded functions. As a consequence, under mild smallness assumption of L_4 both the elliptic problem (1.9) and the parabolic problem (1.10) admit unique smooth solutions by direct methods in classical PDE theory. As Q approaches its physical boundary, both the elliptic and parabolic equations become tensor-valued variational obstacle problems, while both f and $\partial f/\partial Q$ tends to infinity. Therefore, it is an indispensable step to achieve their blowup rates for the corresponding PDE analysis in both the elliptic and the parabolic problems, which is a fundamental issue to be solved.

Motivated by all the existing work, especially the aforementioned studies in both static and dynamic configurations, as well as future consideration of numerical approximations (see Remark 1.3 for details), in this paper we revisit the singular potential f, and aim to establish the blowup rates of $f(Q)$, as well as its gradient $\nabla f(Q)$ near the physical boundary of Q. In view of (1.6), here and after we always assume Q is physical, in the sense that

$$-\frac{1}{3} < \lambda_i(Q) < \frac{2}{3}, \quad 1 \le i \le 3. \tag{1.11}$$

First, we provide a result regarding the blowup rate of $f(Q)$ as Q approaches its physical boundary.

Theorem 1.1 *For any physical Q-tensor, assume $\lambda_1(Q) \le \lambda_2(Q) \le \lambda_3(Q)$. Then the functional f defined in (1.6) is bounded above by*

$$f(Q) \le -\ln 8\sqrt{3} - \frac{1}{2}\ln\Big(\lambda_1(Q) + \frac{1}{3}\Big) - \frac{1}{2}\ln\Big(\lambda_2(Q) + \frac{1}{3}\Big). \tag{1.12}$$

Furthermore, there exists a small computable constant $\delta_0 > 0$, whenever Q approaches its physical boundary in the sense that $\lambda_2(Q) + 1/3 < \delta_0$, it holds

$$\ln 16 - 8\ln\pi - \frac{\pi^5}{16} - \frac{1}{2}\ln\left(\lambda_1(Q) + \frac{1}{3}\right) - \frac{1}{2}\ln\left(\lambda_2(Q) + \frac{1}{3}\right) \le f(Q). \quad (1.13)$$

Remark 1.1 It is noted that the result in Theorem 1.1 is consistent with

$$\frac{1}{2}\ln\left[\frac{1}{(2\pi)^3 e\big(\lambda_1(Q) + \frac{1}{3}\big)}\right] \le f(Q) \le \ln\left[\frac{1}{\lambda_1(Q) + \frac{1}{3}}\right] \quad (1.14)$$

obtained by Ball and Majumdar which is described in Ball (2018) and will appear in Ball and Majumdar (2010).

Remark 1.2 Note that the upper bound in Theorem 1.1 applies to any physical Q-tensor, while the lower bound is valid when $\lambda_2(Q)$ gets close to $-1/3$ (which automatically implies $\lambda_1(Q)$ gets close to $-1/3$). Theorem 1.1 indicates that as Q approaches its physical boundary in the uniaxial direction

$$Q = \begin{pmatrix} -\frac{1}{3} + \varepsilon & 0 & 0 \\ 0 & -\frac{1}{3} + \varepsilon & 0 \\ 0 & 0 & \frac{2}{3} - 2\varepsilon \end{pmatrix}, \qquad \varepsilon \ll 1,$$

$f(Q)$ blows up in the order of $-\ln(\lambda_1(Q) + 1/3)$. Alternatively, when Q is "near" the uniaxial direction, that is, if $\lambda_2(Q)$ is close (but not equal) to $\lambda_1(Q)$, then any blowup order of $-\alpha\ln(\lambda_1(Q) + 1/3)$, $1/2 < \alpha < 1$ could be attained. On the other hand, when $\lambda_2(Q)$ stays away from $-1/3$, $f(Q)$ is of the order $-1/2\ln(\lambda_1(Q) + 1/3)$ as $\lambda_1(Q)$ approaches $-1/3$.

Remark 1.3 Theorem 1.1 will be of significance for numerics as well, because it implies that the function

$$f(Q) + \frac{1}{2}\ln\left(\lambda_1(Q) + \frac{1}{3}\right) + \frac{1}{2}\ln\left(\lambda_2(Q) + \frac{1}{3}\right)$$

is a well-defined, bounded function in the domain of λ_1, λ_2. Hence, by interpolating this well-defined function, we can obtain an accurate numerical approximation of $f(Q)$.

Moreover, the next theorem gives a precise blowup rate of ∇f near the physical boundary of Q.

Theorem 1.2 *For any physical Q-tensor, assume $\lambda_1(Q) \le \lambda_2(Q) \le \lambda_3(Q)$. Then there exists a small computable constant $\varepsilon_0 > 0$, whenever $\lambda_1(Q) + 1/3 < \varepsilon_0$, the* *gradient of the functional f defined in (1.6) satisfies*

$$\frac{C_1}{\lambda_1(Q)+\frac{1}{3}} \le \left|\nabla_{\mathbb{Q}} f(Q)\right| \le \frac{C_2}{\lambda_1(Q)+\frac{1}{3}}, \tag{1.15}$$

with the constants C_1 and C_2 given by

$$C_1 = \frac{\sqrt{3}}{9\sqrt{2\pi e}} \cdot \inf_{\xi\ge 0} \frac{e^{-\xi}\mathrm{I}_0(\xi)}{e^{\frac{-\xi}{2}}\mathrm{I}_0(\frac{\xi}{2})} > 0, \qquad C_2 = \sqrt{6\pi e}\cdot \sup_{\xi\ge 0} \frac{\exp\big(-\frac{\xi}{4}\big)\mathrm{I}_0\big(\frac{\xi}{4}\big)}{\exp\big(-\frac{\xi}{2}\big)\mathrm{I}_0\big(\frac{\xi}{2}\big)}. \tag{1.16}$$

Here

$$\nabla_{\mathbb{Q}} f = \frac{\partial f}{\partial Q} - \frac{1}{3}\operatorname{tr}\big(\frac{\partial f}{\partial Q}\big)\mathbb{I}_3,$$

and $\mathrm{I}_0(\cdot)$ is the zeroth-order modified Bessel function of first kind.

Remark 1.4 We want to point out that (1.15) is consistent with

$$\frac{1}{2}\sqrt{\frac{3}{2}}\ln\Big[\frac{2}{\pi e\big(\lambda_1(Q)+\frac{1}{3}\big)}\Big] \le \left|\nabla_{\mathbb{Q}} f(Q)\right| \le \frac{1}{\lambda_1(Q)+\frac{1}{3}}\ln\Big[\frac{1}{2\pi^3 e\big(\lambda_1(Q)+\frac{1}{3}\big)}\Big], \tag{1.17}$$

that is obtained by Ball and Majumdar in Ball (2018) and will also appear in Ball and Majumdar (2010).

This paper is organized as follows. In Sect. 2, we present a proof of Theorem 1.1. Then, in Sect. 3, we give a proof of Theorem 1.2.

2 Blowup Rate of *f*

Note that (1.11) is equivalent to $Q \in \mathcal{D}(f)$, namely the effective domain of f where f assumes finite values. As proved in Feireisl et al. (2014), f is smooth for $Q \in \mathcal{D}(f)$. Since f is rotation invariant (Ball 2012), here and after, we always assume that any considered physical Q-tensor is diagonal:

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

Note that as Q approaches its physical boundary, we have $\lambda_1 \to -1/3$.

Correspondingly the optimal density function $\rho_Q \in \mathcal{A}_Q$ that satisfies $f(Q) = \int_{\mathbb{S}^2} \rho_Q \ln \rho_Q \,\mathrm{d}S$ is given by (Ball 2012; Ball and Majumdar 2010)

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

Here in (2.2), $Z(\mu_1, \mu_2, \mu_3)$ 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

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

To begin with, we have

Lemma 2.1 *For any physical Q-tensor (2.1), its optimal probability density ρ_Q defined in (2.2) satisfies*

$$\mu_1 \le \mu_2 \le \mu_3.$$

And $\mu_i = \mu_j$ provided $\lambda_i = \lambda_j$ for $1 \le i \ne j \le 3$.

Proof By symmetry, it suffices to prove that μ_i is strictly increasing in λ_i, i.e., $\mu_1 < \mu_2$ whenever $\lambda_1 < \lambda_2$.

Consider eigenvalues $\lambda_1 < \lambda_2$. Then it holds

$$\int_{\mathbb{S}^2} x^2 \rho_Q\, \mathrm{d}S = \lambda_1 + \frac{1}{3} < \lambda_2 + \frac{1}{3} = \int_{\mathbb{S}^2} y^2 \rho_Q\, \mathrm{d}S \tag{2.5}$$

From (2.2) we get

$$\begin{aligned}\rho_Q &= \frac{\exp\left\{\mu_1 x^2 + \mu_2 y^2 - (\mu_1+\mu_2)(1-x^2-y^2)\right\}}{\int_{\mathbb{S}^2} \exp(\mu_1 x^2 + \mu_2 y^2 - (\mu_1+\mu_2)(1-x^2-y^2))\, \mathrm{d}S} \\ &= m^* \exp\left\{(2\mu_1+\mu_2)x^2 + (\mu_1+2\mu_2)y^2\right\},\end{aligned}$$

where

$$m^* = \frac{1}{\int_{\mathbb{S}^2} \exp\left\{(2\mu_1+\mu_2)x^2 + (\mu_1+2\mu_2)y^2\right\} \mathrm{d}S} \tag{2.6}$$

Assume, by contradiction, that $\mu_1 \ge \mu_2$. Using spherical coordinates

$$\begin{cases} x = \sin\theta\cos\phi \\ y = \sin\theta\sin\phi \\ z = \cos\theta \end{cases} \qquad 0 \le \phi < 2\pi,\ 0 \le \theta \le \pi,$$

we get from (2.5) that

$$\begin{aligned}&\lambda_1 - \lambda_2 \\ &= \int_{\mathbb{S}^2} x^2 \rho_Q\, \mathrm{d}S - \int_{\mathbb{S}^2} y^2 \rho_Q\, \mathrm{d}S \\ &= 8m^* \int_0^{\frac{\pi}{2}} \int_0^{\frac{\pi}{2}} (\cos^2\phi - \sin^2\phi) \exp\left\{(\mu_1-\mu_2)\sin^2\theta\cos^2\phi\right\} \mathrm{d}\phi \exp\left\{(\mu_1+2\mu_2)\sin^2\theta\right\} \sin^3\theta\, \mathrm{d}\theta\end{aligned}$$

$$
\begin{aligned}
&= 8m^*\Big[\int_0^{\frac{\pi}{2}}\int_0^{\frac{\pi}{4}}(\cos^2\phi-\sin^2\phi)\exp\big\{(\mu_1-\mu_2)\sin^2\theta\cos^2\phi\big\}\,\mathrm{d}\phi\exp\big\{(\mu_1+2\mu_2)\sin^2\theta\big\}\sin^3\theta\,\mathrm{d}\theta\\
&+\int_0^{\frac{\pi}{2}}\underbrace{\int_{\frac{\pi}{4}}^{\frac{\pi}{2}}(\cos^2\phi-\sin^2\phi)\exp\big\{(\mu_1-\mu_2)\sin^2\theta\cos^2\phi\big\}\,\mathrm{d}\phi}_{\psi=\frac{\pi}{2}-\phi}\exp\big\{(\mu_1+2\mu_2)\sin^2\theta\big\}\sin^3\theta\,\mathrm{d}\theta\Big]\\
&= 8m^*\int_0^{\frac{\pi}{2}}\int_0^{\frac{\pi}{4}}(\cos^2\phi-\sin^2\phi)\underbrace{\big(\exp\big\{(\mu_1-\mu_2)\sin^2\theta\cos^2\phi\big\}-\exp\big\{(\mu_1-\mu_2)\sin^2\theta\sin^2\phi\big\}\big)}_{\geq 0}\,\mathrm{d}\phi\\
&\quad\exp\big\{(\mu_1+2\mu_2)\sin^2\theta\big\}\sin^3\theta\,\mathrm{d}\theta\\
&\geq 0
\end{aligned}
$$

due to the assumption that $\mu_1 \geq \mu_2$, which contradicts the fact that $\lambda_1 < \lambda_2$. □

Next we can see that the index μ_1 in (2.2) satisfies

Lemma 2.2 *As* $\lambda_1 \to -\frac{1}{3}$, $\mu_1 \to -\infty$.

Proof First, observe that

$$
\begin{aligned}
\frac{\partial\ln(\lambda_1+\frac{1}{3})}{\partial\mu_1} &= \frac{\partial}{\partial\mu_1}\Big[\ln\int_{\mathbb{S}^2}x^2\exp(\mu_1x^2+\mu_2y^2+\mu_3z^2)\,\mathrm{d}S-\ln Z(\mu_1,\mu_2,\mu_3)\Big]\\
&= \frac{\int_{\mathbb{S}^2}x^4\exp(\mu_1x^2+\mu_2y^2+\mu_3z^2)\,\mathrm{d}S}{\int_{\mathbb{S}^2}x^2\exp(\mu_1x^2+\mu_2y^2+\mu_3z^2)\,\mathrm{d}S}-\Big(\lambda_1+\frac{1}{3}\Big)\\
&= \Big(\lambda_1+\frac{1}{3}\Big)^{-1}\Big[\int_{\mathbb{S}^2}x^4\rho_Q\,\mathrm{d}S\underbrace{\int_{\mathbb{S}^2}\rho_Q\,\mathrm{d}S}_{=1}-\Big(\int_{\mathbb{S}^2}x^2\rho_Q\,\mathrm{d}S\Big)^2\Big] > 0
\end{aligned}
$$

due to Schwarz's inequality, and the fact that ρ_Q is not a perfect alignment of molecules as Q approaches the physical boundary. Hence, as $\lambda_1 \searrow -1/3$, μ_1 is strictly decreasing. It remains to prove μ_1 is unbounded as $\lambda_1 \to -1/3$. Suppose there exists a constant $M > 0$, such that $\mu_1 \geq -M$ as $\lambda_1 \to -1/3$, then by (2.2) and Lemma 2.1 we see that $-M \leq \mu_1 \leq \mu_2 \leq \mu_3 \leq 2M$. As a consequence, together with the basic inequality

$$
\frac{2\theta}{\pi} \leq \sin\theta < \theta, \quad \forall\, 0 < \theta \leq \frac{\pi}{2}, \tag{2.7}
$$

we obtain

$$
\begin{aligned}
\lambda_1+\frac{1}{3} &= \int_{\mathbb{S}^2}x^2\rho_Q\,\mathrm{d}S = \frac{\int_{\mathbb{S}^2}x^2\exp\big\{(2\mu_1+\mu_2)x^2+(\mu_1+2\mu_2)y^2\big\}\,\mathrm{d}S}{\int_{\mathbb{S}^2}\exp\big\{\underbrace{(2\mu_1+\mu_2)}_{\leq 0}x^2+\underbrace{(\mu_1+2\mu_2)}_{\leq 0}y^2\big\}\,\mathrm{d}S}\\
&\geq \frac{\int_{\mathbb{S}^2}x^2\exp\big\{-3M(x^2+y^2)\big\}\,\mathrm{d}S}{\int_{\mathbb{S}^2}\,\mathrm{d}S} = \frac{8\int_0^{\frac{\pi}{2}}\cos^2\phi\,\mathrm{d}\phi\int_0^{\frac{\pi}{2}}\exp\big\{-3M\sin^2\theta\big\}\sin^3\theta\,\mathrm{d}\theta}{4\pi}\\
&\geq \frac{2\pi\frac{8}{\pi^3}\int_0^{\frac{\pi}{2}}\exp(-3M\theta^2)\theta^3\,\mathrm{d}\theta}{4\pi} \geq \frac{4}{\pi^3}\exp\Big(\frac{-3M\pi^2}{4}\Big)\int_0^{\frac{\pi}{2}}\theta^3\,\mathrm{d}\theta = \frac{\pi}{16}\exp\Big(\frac{-3M\pi^2}{4}\Big),
\end{aligned}
$$

which is a contradiction. Therefore, such lower bound $-M$ cannot exist, and the proof is complete. □

Remark 2.1 It follows from the proof of Lemma 2.2 that in order to ensure $\mu_1 < -M$ for any $M > 0$, it suffices to assume

$$\lambda_1(Q) + \frac{1}{3} < \frac{\pi}{16} \exp\Big(\frac{-3M\pi^2}{4}\Big).$$

Now we are ready to prove Theorem 1.1.

2.1 Proof of Upper Bound of *f*

Proof To this end, we consider Q of the form

$$Q = \begin{pmatrix} -\frac{1}{3} + \frac{\varepsilon^2}{3} & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}, \qquad -\frac{1}{3} + \frac{\varepsilon^2}{3} \leq \lambda_2 \leq \lambda_3, \ 0 < \varepsilon \leq 1. \tag{2.8}$$

Using the coordinate system

$$\begin{cases} x = \cos\theta \\ y = \sin\theta \sin\phi \\ z = \sin\theta\cos\phi \end{cases} \qquad 0 \leq \phi < 2\pi, \ 0 \leq \theta \leq \pi,$$

we consider the domain

$$\begin{aligned} S^* \overset{\text{def}}{=} \big\{(1, \phi, \theta) \in \mathbb{S}^2 \big| \ \phi \in [0, b] \cup [\pi - b, \pi] \cup [\pi, \pi + b] \cup [2\pi - b, 2\pi], \\ \theta \in [\arccos\varepsilon, \pi - \arccos\varepsilon]\big\}, \end{aligned} \tag{2.9}$$

where $0 < b \leq \pi/2$ is to be determined. Meanwhile, let

$$\rho_\varepsilon = \frac{1}{8b\varepsilon}\chi_{S^*}.$$

Then it is easy to check

$$\int_{\mathbb{S}^2} \rho_\varepsilon \, \mathrm{d}S = \frac{4}{8b\varepsilon}\int_0^b \mathrm{d}\phi \int_{\arccos\varepsilon}^{\pi - \arccos\varepsilon} \sin\theta \, \mathrm{d}\theta = 1,$$

and the second moments with respect to ρ_ε are given by

$$\int_{\mathbb{S}^2} x^2 \rho_\varepsilon \, \mathrm{d}S = \frac{1}{b\varepsilon}\int_0^b \mathrm{d}\phi \int_{\arccos\varepsilon}^{\frac{\pi}{2}} \cos^2\theta \sin\theta \, \mathrm{d}\theta = \frac{\varepsilon^2}{3},$$

$$
\begin{aligned}
\int_{\mathbb{S}^2} y^2\rho_\varepsilon \,\mathrm{d}S &= \frac{1}{b\varepsilon}\int_0^b \sin^2\phi \,\mathrm{d}\phi \int_{\arccos\varepsilon}^{\frac{\pi}{2}} \sin^3\theta \,\mathrm{d}\theta = \frac{1}{b\varepsilon}\Big(\frac{b}{2}-\frac{\sin 2b}{4}\Big)\Big(\varepsilon-\frac{\varepsilon^3}{3}\Big)\\
&= \Big(\frac{1}{2}-\frac{\sin 2b}{4b}\Big)\Big(1-\frac{\varepsilon^2}{3}\Big),\\
\int_{\mathbb{S}^2} z^2\rho_\varepsilon \,\mathrm{d}S &= \frac{1}{b\varepsilon}\int_0^b \cos^2\phi \,\mathrm{d}\phi \int_{\arccos\varepsilon}^{\frac{\pi}{2}} \sin^3\theta \,\mathrm{d}\theta = \frac{1}{b\varepsilon}\Big(\frac{b}{2}+\frac{\sin 2b}{4}\Big)\Big(\varepsilon-\frac{\varepsilon^3}{3}\Big)\\
&= \Big(\frac{1}{2}+\frac{\sin 2b}{4b}\Big)\Big(1-\frac{\varepsilon^2}{3}\Big),\\
\int_{\mathbb{S}^2} xy\rho_\varepsilon \,\mathrm{d}S &= \int_{\mathbb{S}^2} yz\rho_\varepsilon \,\mathrm{d}S = \int_{\mathbb{S}^2} zx\rho_\varepsilon \,\mathrm{d}S = 0.
\end{aligned}
$$

Therefore, $\rho_\varepsilon \in \mathcal{A}_R$ with

$$
R = \begin{pmatrix} -\frac{1}{3}+\frac{\varepsilon^2}{3} & 0 & 0 \\ 0 & \frac{1}{6}-\frac{\sin 2b}{4b}-(\frac{1}{2}-\frac{\sin 2b}{4b})\frac{\varepsilon^2}{3} & 0 \\ 0 & 0 & \frac{1}{6}+\frac{\sin 2b}{4b}-(\frac{1}{2}+\frac{\sin 2b}{4b})\frac{\varepsilon^2}{3} \end{pmatrix}
$$

We need to find a suitable $0 < b \le \pi/2$, such that

$$
\frac{1}{6}-\frac{\sin 2b}{4b}-\Big(\frac{1}{2}-\frac{\sin 2b}{4b}\Big)\frac{\varepsilon^2}{3} = \lambda_2,
$$

which is equivalent to

$$
\frac{\sin 2b}{2b} = 1-\frac{2\big(\lambda_2+\frac{1}{3}\big)}{1-\frac{\varepsilon^2}{3}}. \tag{2.10}
$$

Note that $\sin(x)/x$ is monotone decreasing in $(0,\pi]$, with

$$
\lim_{x\to 0^+}\frac{\sin x}{x} = 1,
$$

hence we know (2.10) is solvable with $b \in (0, \pi/2]$. As a consequence, $R = Q$ and using mean value theorem we get

$$
x-\frac{x^3}{6} < \sin x, \quad \forall\, 0 < x \le \pi; \qquad \frac{1}{1-y} > 1+y, \quad \forall\, 0 < y < 1.
$$

Hence, after inserting $x = 2b$, $y = \varepsilon^2/3$ into (2.10) we obtain

$$
1-\frac{2b^2}{3} < \frac{\sin 2b}{2b} < 1-2\Big(1+\frac{\varepsilon^2}{3}\Big)\Big(\lambda_2+\frac{1}{3}\Big), \tag{2.11}
$$

which further implies

$$b^2 > (3+\varepsilon^2)\Big(\lambda_2 + \frac{1}{3}\Big) > 3\Big(\lambda_2 + \frac{1}{3}\Big). \tag{2.12}$$

In conclusion, we see $\rho_\varepsilon \in \mathcal{A}_Q$ for Q defined in (2.8), where $\lambda_1(Q) + 1/3 = \varepsilon^2/3$, and

$$\begin{aligned} f(Q) &\le \int_{\mathbb{S}^2} \rho_\varepsilon \log \rho_\varepsilon \,\mathrm{d}S \le \frac{8}{8b\varepsilon}\int_0^b \mathrm{d}\phi \int_{\arccos\varepsilon}^{\frac{\pi}{2}} \ln\frac{1}{8b\varepsilon}\sin\theta\,\mathrm{d}\theta = \ln\frac{1}{8b\varepsilon} = -\ln 8 - \ln b - \ln\varepsilon \\ &\le -\ln 8\sqrt{3} - \frac{1}{2}\ln\Big(\lambda_1(Q) + \frac{1}{3}\Big) - \frac{1}{2}\ln\Big(\lambda_2(Q) + \frac{1}{3}\Big). \end{aligned} \tag{2.13}$$

2.2 Proof of Lower Bound of *f*

There is no doubt that the proof of lower bound (1.13) is far more difficult than that of (1.12), because we can no longer utilize any specific probability density ρ in the admissible set $\mathcal{A}_Q$. To accomplish the goal, more delicate analysis is needed.

In this subsection we denote

$$\varepsilon = \lambda_1(Q) + \frac{1}{3}, \qquad \delta = \lambda_2(Q) + \frac{1}{3}. \tag{2.14}$$

By (2.2)-(2.4), we get

$$\varepsilon = \frac{\int_{\mathbb{S}^2} x^2 \exp(\mu_1 x^2 + \mu_2 y^2 + \mu_3 z^2)\,\mathrm{d}S}{\int_{\mathbb{S}^2} \exp(\mu_1 x^2 + \mu_2 y^2 + \mu_3 z^2)\,\mathrm{d}S} = \frac{\int_{\mathbb{S}^2} x^2 \exp(-\nu_1 x^2 - \nu_2 y^2)\,\mathrm{d}S}{\int_{\mathbb{S}^2} \exp(-\nu_1 x^2 - \nu_2 y^2)\,\mathrm{d}S}, \tag{2.15}$$

$$\delta = \frac{\int_{\mathbb{S}^2} y^2 \exp(\mu_1 x^2 + \mu_2 y^2 + \mu_3 z^2)\,\mathrm{d}S}{\int_{\mathbb{S}^2} \exp(\mu_1 x^2 + \mu_2 y^2 + \mu_3 z^2)\,\mathrm{d}S} = \frac{\int_{\mathbb{S}^2} y^2 \exp(-\nu_1 x^2 - \nu_2 y^2)\,\mathrm{d}S}{\int_{\mathbb{S}^2} \exp(-\nu_1 x^2 - \nu_2 y^2)\,\mathrm{d}S}, \tag{2.16}$$

where

$$\nu_1 = -(2\mu_1 + \mu_2), \quad \nu_2 = -(\mu_1 + 2\mu_2). \tag{2.17}$$

By (2.2) and Lemma 2.1, we see

$$\nu_1 \ge \nu_2 = \mu_3 - \mu_2 \ge 0. \tag{2.18}$$

Besides, it follows from (2.2), Lemma 2.1 and Lemma 2.2 that

$$\nu_1 = -\mu_1 + \mu_3 \ge -\mu_1 \to +\infty, \quad \text{as } \varepsilon \to 0. \tag{2.19}$$

Actually, we can establish a stronger result in the following sense

Lemma 2.3 *There exists a small computable constant* $\delta_0 > 0$ *such that*

$$\delta \geq \frac{(2e-5)}{24e} e^{-\nu_2}, \qquad \forall\, \delta < \delta_0. \tag{2.20}$$

As a consequence,

$$\nu_1 \geq \nu_2 \geq -\ln\delta + \ln\Big[\frac{(2e-5)}{24e}\Big], \qquad \forall\, \delta < \delta_0. \tag{2.21}$$

Proof Using (2.16) and (2.18) we have

$$\delta \geq \frac{\int_{\mathbb{S}^2} y^2 \exp(-\nu_1 x^2 - \nu_2)\,\mathrm{d}S}{\int_{\mathbb{S}^2} \exp(-\nu_1 x^2)\,\mathrm{d}S} = e^{-\nu_2} \frac{\int_{\mathbb{S}^2} y^2 \exp(-\nu_1 x^2)\,\mathrm{d}S}{\int_{\mathbb{S}^2} \exp(-\nu_1 x^2)\,\mathrm{d}S}. \tag{2.22}$$

We proceed to estimate the numerator and denominator of R.H.S. in (2.22), respectively. By Remark 2.1,

$$\nu_1 \geq -\mu_1 > \frac{4}{\pi^2}, \qquad \text{provided } \delta < \frac{\pi}{16e^3}.$$

Together with (2.7) and spherical coordinates

$$\begin{cases} x = \sin\theta\cos\phi, \\ y = \sin\theta\sin\phi, \\ z = \cos\theta, \end{cases} \qquad 0 \leq \theta \leq \pi,\ 0 \leq \phi < 2\pi,$$

we have

$$\begin{aligned} \int_{\mathbb{S}^2} \exp(-\nu_1 x^2)\,\mathrm{d}S &= 2\int_0^{2\pi}\int_0^{\frac{\pi}{2}} \sin\theta e^{-\nu_1 \sin^2\theta\cos^2\phi}\,\mathrm{d}\theta\mathrm{d}\phi \leq 2\int_0^{2\pi}\int_0^{\frac{\pi}{2}} \theta e^{-\frac{4}{\pi^2}\nu_1\theta^2\cos^2\phi}\,\mathrm{d}\theta\mathrm{d}\phi \\ &= \frac{\pi^2}{4}\int_0^{2\pi} \frac{1-e^{-\nu_1\cos^2\phi}}{\nu_1\cos^2\phi}\,\mathrm{d}\phi = \pi^2\int_0^{\frac{\pi}{2}} \frac{1-e^{-\nu_1\sin^2\phi}}{\nu_1\sin^2\phi}\,\mathrm{d}\phi \\ &\leq 4\underbrace{\int_0^{\frac{1}{\sqrt{\nu_1}}} \frac{1-e^{-\nu_1\phi^2}}{\nu_1\phi^2}\,\mathrm{d}\phi}_{:=J_1} + 4\underbrace{\int_{\frac{1}{\sqrt{\nu_1}}}^{\frac{\pi}{2}} \frac{1}{\nu_1\phi^2}\,d\phi}_{:=J_2}. \end{aligned}$$

Note that

$$\sup_{\phi\in(0,1/\sqrt{\nu_1})} \frac{1-e^{-\nu_1\phi^2}}{\nu_1\phi^2} = 1 \implies J_1 \leq \frac{1}{\sqrt{\nu_1}}, \quad \text{and} \quad J_2 = \frac{\sqrt{\nu_1}-\frac{2}{\pi}}{\nu_1} \leq \frac{1}{\sqrt{\nu_1}}.$$

Hence,

$$\int_{\mathbb{S}^2} \exp(-\nu_1 x^2)\,\mathrm{d}S \leq \frac{8}{\sqrt{\nu_1}}. \tag{2.23}$$

Meanwhile, using (2.7) and integration by parts we obtain

$$\begin{aligned}
&\int_{\mathbb{S}^2} y^2 \exp(-\nu_1 x^2)\,\mathrm{d}S \\
&= 2\int_0^{2\pi} \sin^2\phi \int_0^{\frac{\pi}{2}} \sin^3\theta e^{-\nu_1 \sin^2\theta\cos^2\phi}\,\mathrm{d}\theta\mathrm{d}\phi \\
&\geq 2\Big(\frac{2}{\pi}\Big)^3 \int_0^{2\pi} \sin^2\phi \int_0^{\frac{\pi}{2}} \theta^3 e^{-\nu_1\theta^2\cos^2\phi}\,\mathrm{d}\theta\mathrm{d}\phi \\
&= \Big(\frac{4}{\pi}\Big)^3 \int_0^{2\pi} \frac{\sin^2\phi}{2\nu_1^2\cos^4\phi}\Big[1-\Big(\frac{\pi^2}{4}\nu_1\cos^2\phi+1\Big)\exp\Big(-\frac{\pi^2}{4}\nu_1\cos^2\phi\Big)\Big]\,\mathrm{d}\phi \\
&= \Big(\frac{4}{\pi}\Big)^3 \int_0^{2\pi} \frac{\cos^2\phi}{2\nu_1^2\sin^4\phi}\Big[1-\Big(\frac{\pi^2}{4}\nu_1\sin^2\phi+1\Big)\exp\Big(-\frac{\pi^2}{4}\nu_1\sin^2\phi\Big)\Big]\,\mathrm{d}\phi.
\end{aligned} \tag{2.24}$$

Note that

$$\frac{\mathrm{d}}{\mathrm{d}z}\Big[\Big(\frac{\pi^2}{4}\nu_1 z+1\Big)e^{-\frac{\pi^2}{4}\nu_1 z}\Big] = -\frac{\pi^2}{4}\nu_1 z e^{-\frac{\pi^2}{4}\nu_1 z} \leq 0, \qquad \forall z \geq 0.$$

Hence,

$$1-\Big(\frac{\pi^2}{4}\nu_1\sin^2\phi+1\Big)\exp\Big(-\frac{\pi^2}{4}\nu_1\sin^2\phi\Big) \geq 0, \qquad \forall \phi \in [0, 2\pi),$$

and (2.24) continues as

$$\begin{aligned}
&\int_{\mathbb{S}^2} y^2 \exp(-\nu_1 x^2)\,\mathrm{d}S \\
&\geq \Big(\frac{4}{\pi}\Big)^3 \int_{\frac{2}{\pi\sqrt{\nu_1}}}^{\frac{\pi}{4}} \frac{\cos^2\phi}{2\nu_1^2\sin^4\phi}\Big[1-\Big(\frac{\pi^2}{4}\nu_1\sin^2\phi+1\Big)\exp\Big(-\frac{\pi^2}{4}\nu_1\sin^2\phi\Big)\Big]\,\mathrm{d}\phi \\
&\geq \Big(\frac{4}{\pi}\Big)^3 \int_{\frac{2}{\pi\sqrt{\nu_1}}}^{\frac{\pi}{4}} \frac{1}{4\nu_1^2\sin^4\phi}\Big[1-\Big(\frac{\pi^2}{4}\nu_1\sin^2\phi+1\Big)\exp\Big(-\frac{\pi^2}{4}\nu_1\sin^2\phi\Big)\Big]\,\mathrm{d}\phi \\
&\geq \Big(\frac{4}{\pi}\Big)^3 \int_{\frac{2}{\pi\sqrt{\nu_1}}}^{\frac{\pi}{4}} \frac{1}{4\nu_1^2\sin^4\phi}\Big[1-\Big(\frac{\pi^2}{4}\nu_1\sin^2\frac{2}{\pi\sqrt{\nu_1}}+1\Big)\exp\Big(-\frac{\pi^2}{4}\nu_1\sin^2\frac{2}{\pi\sqrt{\nu_1}}\Big)\Big]\,\mathrm{d}\phi \\
&\geq \Big(\frac{4}{\pi}\Big)^3 \int_{\frac{2}{\pi\sqrt{\nu_1}}}^{\frac{\pi}{4}} \frac{1}{4\nu_1^2\sin^4\phi}\Big[1-2\exp\Big(-\frac{\pi^2}{4}\nu_1\sin^2\frac{2}{\pi\sqrt{\nu_1}}\Big)\Big]\,\mathrm{d}\phi.
\end{aligned} \tag{2.25}$$

By (2.19),

$$\lim_{\delta\to 0}\exp\Big(-\frac{\pi^2}{4}\nu_1\sin^2\frac{2}{\pi\sqrt{\nu_1}}\Big) = \lim_{\nu_1\to\infty}\exp\Big(-\frac{\pi^2}{4}\nu_1\sin^2\frac{2}{\pi\sqrt{\nu_1}}\Big) = \frac{1}{e}.$$

Thus, by Remark 2.1 there exists a small computable constant $\delta_0 > 0$, such that

$$1 - 2\exp\Big(-\frac{\pi^2}{4}\nu_1 \sin^2\frac{2}{\pi\sqrt{\nu_1}}\Big) \geq 1 - \frac{5}{2e}, \qquad \forall\,\delta < \delta_0.$$

This further implies

$$\int_{\mathbb{S}^2} y^2 \exp(-\nu_1 x^2)\,\mathrm{d}S \geq \Big(1-\frac{5}{2e}\Big)\Big(\frac{4}{\pi}\Big)^3 \int_{\frac{2}{\pi\sqrt{\nu_1}}}^{\frac{\pi}{4}} \frac{1}{4\nu_1^2 \sin^4\phi}\,\mathrm{d}\phi \geq \Big(1-\frac{5}{2e}\Big)\Big(\frac{4}{\pi}\Big)^3 \int_{\frac{2}{\pi\sqrt{\nu_1}}}^{\frac{\pi}{4}} \frac{1}{4\nu_1^2\phi^4}\,\mathrm{d}\phi$$
$$\geq \frac{2e-5}{3e\sqrt{\nu_1}}, \qquad \forall\,\delta < \delta_0. \tag{2.26}$$

To sum up, we conclude

$$\delta \geq e^{-\nu_2}\frac{\int_{\mathbb{S}^2} y^2\exp(-\nu_1x^2)\,\mathrm{d}S}{\int_{\mathbb{S}^2}\exp(-\nu_1x^2)\,\mathrm{d}S} \geq e^{-\nu_2}\frac{(2e-5)}{3e\sqrt{\nu_1}}\Big/\frac{8}{\sqrt{\nu_1}}$$
$$= \frac{(2e-5)}{24e}e^{-\nu_2}, \qquad \forall\,\delta < \delta_0,$$

completing the proof. □

Remark 2.2 Lemma 2.3 implies that as $\lambda_2(Q) \to -1/3$, that is $\delta \to 0^+$, we have both $\nu_1, \nu_2 \to +\infty$.

Next, we denote

$$A(\phi) = \nu_1\cos^2\phi + \nu_2\sin^2\phi, \qquad 0 \leq \phi < 2\pi. \tag{2.27}$$

We can establish the following estimates

Lemma 2.4 *There exists a small computable constant $\delta_0 > 0$ such that*

$$\frac{1}{\pi}\int_0^{2\pi}\frac{1}{A(\phi)}\,\mathrm{d}\phi \leq \int_{\mathbb{S}^2}\exp(-\nu_1x^2-\nu_2y^2)\,\mathrm{d}S \leq \frac{\pi^2}{4}\int_0^{2\pi}\frac{1}{A(\phi)}\,\mathrm{d}\phi, \qquad \forall\,\delta<\delta_0, \tag{2.28}$$
$$\frac{4}{\pi^3}\int_0^{2\pi}\frac{\cos^2\phi}{A^2(\phi)}\,\mathrm{d}\phi \leq \int_{\mathbb{S}^2}x^2\exp(-\nu_1x^2-\nu_2y^2)\,\mathrm{d}S \leq \frac{\pi^4}{16}\int_0^{2\pi}\frac{\cos^2\phi}{A^2(\phi)}\,\mathrm{d}\phi, \qquad \forall\,\delta<\delta_0, \tag{2.29}$$
$$\frac{4}{\pi^3}\int_0^{2\pi}\frac{\sin^2\phi}{A^2(\phi)}\,\mathrm{d}\phi \leq \int_{\mathbb{S}^2}y^2\exp(-\nu_1x^2-\nu_2y^2)\,\mathrm{d}S \leq \frac{\pi^4}{16}\int_0^{2\pi}\frac{\sin^2\phi}{A^2(\phi)}\,\mathrm{d}\phi, \qquad \forall\,\delta<\delta_0. \tag{2.30}$$

Proof To begin with, by (2.18) we have

$$A(\phi) \geq \nu_2\cos^2\phi + \nu_2\sin^2\phi = \nu_2.$$

This together with Lemma 2.3 implies that there exists a small computable constant $\delta_0 > 0$ such that

$$e^{\frac{-\pi^2 A(t)}{4}} \leq e^{\frac{-\pi^2 \nu_2}{4}} \leq \frac{1}{2} - \frac{1}{e}, \qquad \forall\, \delta < \delta_0. \tag{2.31}$$

Using (2.7) and integration by parts, we obtain

$$\begin{aligned}\int_{\mathbb{S}^2} \exp(-\nu_1 x^2 - \nu_2 y^2)\,\mathrm{d}S &= 2\int_0^{2\pi}\int_0^{\frac{\pi}{2}} \sin\theta \exp\big[-A(\phi)\sin^2\theta\big]\,\mathrm{d}\theta\mathrm{d}\phi\\ &\leq 2\int_0^{2\pi}\int_0^{\frac{\pi}{2}} \theta \exp\big[-4A(\phi)\pi^{-2}\theta^2\big]\,\mathrm{d}\theta\mathrm{d}\phi\\ &= \int_0^{2\pi} \frac{\pi^2 - \pi^2 e^{-A(\phi)}}{4A(\phi)}\,\mathrm{d}\phi \leq \frac{\pi^2}{4}\int_0^{2\pi}\frac{1}{A(\phi)}\,\mathrm{d}\phi,\end{aligned}$$

and together with (2.31) we have

$$\begin{aligned}\int_{\mathbb{S}^2} \exp(-\nu_1 x^2 - \nu_2 y^2)\,\mathrm{d}S &= 2\int_0^{2\pi}\int_0^{\frac{\pi}{2}} \sin\theta \exp\big[-A(\phi)\sin^2\theta\big]\,\mathrm{d}\theta\mathrm{d}\phi\\ &\geq \frac{4}{\pi}\int_0^{2\pi}\int_0^{\frac{\pi}{2}} \theta \exp\big[-A(\phi)\theta^2\big]\,\mathrm{d}\theta\mathrm{d}\phi\\ &= \frac{2}{\pi}\int_0^{2\pi} \frac{1}{A(\phi)}\big[1 - e^{-A(\phi)\pi^2/4}\big]\,\mathrm{d}\phi\\ &\geq \frac{1}{\pi}\int_0^{2\pi}\frac{1}{A(\phi)}\,\mathrm{d}\phi,\end{aligned}$$

concluding the proof of (2.28).

To proceed, using (2.7) and integration by parts again, we get

$$\begin{aligned}\int_{\mathbb{S}^2} x^2 \exp(-\nu_1 x^2 - \nu_2 y^2)\,\mathrm{d}S &= 2\int_0^{2\pi}\int_0^{\frac{\pi}{2}} \cos^2\phi \sin^3\theta \exp\big[-A(\phi)\sin^2\theta\big]\,\mathrm{d}\theta\mathrm{d}\phi\\ &\leq 2\int_0^{2\pi}\int_0^{\frac{\pi}{2}} \cos^2\phi\ \theta^3 \exp\big[-A(\phi)4\pi^{-2}\theta^2\big]\,\mathrm{d}\theta\mathrm{d}\phi\\ &= \frac{\pi^4}{16}\int_0^{2\pi}\frac{\cos^2\phi}{A^2(\phi)}\Big\{1 - e^{-A(\phi)}\big[A(\phi)+1\big]\Big\}\,\mathrm{d}\phi\\ &\leq \frac{\pi^4}{16}\int_0^{2\pi}\frac{\cos^2\phi}{A^2(\phi)}\,\mathrm{d}\phi\end{aligned}$$

and similarly

$$\begin{aligned}&\int_{\mathbb{S}^2} x^2 \exp(-\nu_1 x^2 - \nu_2 y^2)\,\mathrm{d}S\\ &\quad= 2\int_0^{2\pi}\int_0^{\frac{\pi}{2}} \cos^2\phi \sin^3\theta \exp\big[-A(\phi)\sin^2\theta\big]\,\mathrm{d}\theta\mathrm{d}\phi\end{aligned}$$

$$
\begin{aligned}
&\geq 2\Big(\frac{2}{\pi}\Big)^3 \int_0^{2\pi}\int_0^{\frac{\pi}{2}} \cos^2\phi\, \theta^3 \exp\big[-A(\phi)\theta^2\big]\, \mathrm{d}\theta \mathrm{d}\phi \\
&= \Big(\frac{2}{\pi}\Big)^3 \int_0^{2\pi} \frac{\cos^2\phi}{A^2(\phi)} \Big\{1 - \frac{1}{4} e^{-\pi^2 A(\phi)/4}\big[\pi^2 A(\phi) + 4\big]\Big\}\, \mathrm{d}\phi \\
&= \frac{8}{\pi^3}\int_0^{2\pi} \frac{\cos^2\phi}{A^2(\phi)}\, \mathrm{d}\phi \\
&\quad - \frac{8}{\pi^3} \underbrace{\int_0^{2\pi} \frac{\cos^2\phi}{A^2(\phi)} \frac{\pi^2 A(\phi)}{4} \exp\Big[\frac{-\pi^2 A(\phi)}{4}\Big]\, \mathrm{d}\phi}_{I_1} \\
&\quad - \frac{8}{\pi^3} \underbrace{\int_0^{2\pi} \frac{\cos^2\phi}{A^2(\phi)} \exp\Big[\frac{-\pi^2 A(\phi)}{4}\Big]\, \mathrm{d}\phi}_{I_2}
\end{aligned}
$$

Hence, to attain (2.29), it remains to estimate I_1 and I_2. First, observe that $ze^{-z} \in [0, 1/e]$ for $z \geq 0$, hence

$$
I_1 \leq \frac{1}{e}\int_0^{2\pi} \frac{\cos^2\phi}{A^2(\phi)}\, \mathrm{d}\phi.
$$

Besides, it follows from (2.31) that

$$
I_2 \leq \Big(\frac{1}{2} - \frac{1}{e}\Big)\int_0^{2\pi} \frac{\cos^2\phi}{A^2(\phi)}\, \mathrm{d}\phi.
$$

To sum up, we conclude

$$
\int_{\mathbb{S}^2} x^2 \exp(-\nu_1 x^2 - \nu_2 y^2)\, \mathrm{d}S \geq \frac{4}{\pi^3}\int_0^{2\pi} \frac{\cos^2\phi}{A^2(\phi)}\, \mathrm{d}\phi,
$$

hence the proof of (2.29) is complete. The proof of (2.30) is completely analogous to that of (2.29). ◻

As a matter of fact, all the bounds in Lemma 2.4 can be achieved explicitly in terms of ν_1, ν_2.

Lemma 2.5 *For any $\nu_1, \nu_2 > 0$, the following identities are satisfied:*

$$
\int_0^{2\pi} \frac{1}{A(\phi)}\, \mathrm{d}\phi = 4\int_0^{\frac{\pi}{2}} \frac{1}{A(\phi)}\, \mathrm{d}\phi = \frac{2\pi}{\sqrt{\nu_1\nu_2}}, \tag{2.32}
$$

$$
\int_0^{2\pi} \frac{\sin^2\phi}{A^2(\phi)}\, \mathrm{d}\phi = 4\int_0^{\frac{\pi}{2}} \frac{\sin^2\phi}{A^2(\phi)}\, \mathrm{d}\phi = \frac{\pi}{\nu_2\sqrt{\nu_1\nu_2}}, \tag{2.33}
$$

$$
\int_0^{2\pi} \frac{\cos^2\phi}{A^2(\phi)}\, \mathrm{d}\phi = 4\int_0^{\frac{\pi}{2}} \frac{\cos^2\phi}{A^2(\phi)}\, \mathrm{d}\phi = \frac{\pi}{\nu_1\sqrt{\nu_1\nu_2}}. \tag{2.34}
$$

Proof The proof relies on direct derivation of these anti-derivatives. Note that

$$\int \frac{1}{A(\phi)}\,\mathrm{d}\phi = \int \frac{\sec^2\phi}{\nu_1+\nu_2\tan^2\phi}\,\mathrm{d}\phi = \frac{1}{\sqrt{\nu_1\nu_2}}\int \frac{1}{1+\left(\sqrt{\frac{\nu_2}{\nu_1}}\tan\phi\right)^2}\,\mathrm{d}\left(\sqrt{\frac{\nu_2}{\nu_1}}\tan\phi\right)$$
$$= \frac{1}{\sqrt{\nu_1\nu_2}}\arctan\left(\sqrt{\frac{\nu_2}{\nu_1}}\tan\phi\right)+C.$$

Hence,

$$\int_0^{2\pi}\frac{1}{A(\phi)}\,\mathrm{d}\phi = 4\int_0^{\frac{\pi}{2}}\frac{1}{A(\phi)}\,\mathrm{d}\phi = \frac{4}{\sqrt{\nu_1\nu_2}}\arctan\left(\sqrt{\frac{\nu_2}{\nu_1}}\tan\phi\right)\Big|_0^{\frac{\pi}{2}} = \frac{2\pi}{\sqrt{\nu_1\nu_2}}.$$

Next,

$$\begin{aligned}
&\int \frac{\sin^2\phi}{A^2(\phi)}\,\mathrm{d}\phi\\
&= \int \frac{\tan^2\phi\sec^2\phi}{(\nu_1+\nu_2\tan^2\phi)^2}\,\mathrm{d}\phi = \frac{1}{\nu_2}\int\frac{(\nu_1+\nu_2\tan^2\phi)\sec^2\phi}{(\nu_1+\nu_2\tan^2\phi)^2}\,\mathrm{d}\phi - \frac{\nu_1}{\nu_2}\int\frac{\sec^2\phi}{(\nu_1+\nu_2\tan^2\phi)^2}\,\mathrm{d}\phi\\
&= \frac{1}{\sqrt{\nu_1\nu_2}\nu_2}\int\frac{1}{1+\left(\sqrt{\frac{\nu_2}{\nu_1}}\tan\phi\right)^2}\,\mathrm{d}\left(\sqrt{\frac{\nu_2}{\nu_1}}\tan\phi\right)\\
&\quad - \frac{1}{\sqrt{\nu_1\nu_2}\nu_2}\int\frac{1}{\left[1+\left(\sqrt{\frac{\nu_2}{\nu_1}}\tan\phi\right)^2\right]^2}\,\mathrm{d}\left(\sqrt{\frac{\nu_2}{\nu_1}}\tan\phi\right)\\
&= \frac{1}{\sqrt{\nu_1\nu_2}\nu_2}\arctan\left(\sqrt{\frac{\nu_2}{\nu_1}}\tan\phi\right) - \frac{1}{\sqrt{\nu_1\nu_2}\nu_2}\underbrace{\int\frac{1}{\left[1+\left(\sqrt{\frac{\nu_2}{\nu_1}}\tan\phi\right)^2\right]^2}\,\mathrm{d}\left(\sqrt{\frac{\nu_2}{\nu_1}}\tan\phi\right)}_{I_1}.
\end{aligned}$$

By setting $u=\sqrt{\frac{\nu_2}{\nu_1}}\tan\phi$ we obtain

$$I_1 = \int\frac{1}{(1+u^2)^2}\,\mathrm{d}u \overset{(\theta=\tan u)}{=} \int\cos^2\theta\,\mathrm{d}\theta = \frac{\sin(2\theta)}{4}+\frac{\theta}{2}+C = \frac{1}{2}\frac{u}{1+u^2}+\frac{\arctan u}{2}+C.$$

Thus,

$$\int\frac{\sin^2\phi}{A^2(\phi)}\,\mathrm{d}\phi = \frac{1}{2\sqrt{\nu_1\nu_2}\nu_2}\arctan\left(\sqrt{\frac{\nu_2}{\nu_1}}\tan\phi\right) - \frac{1}{2\nu_2}\frac{\cos\phi\sin\phi}{\nu_1\cos^2\phi+\nu_2\sin^2\phi}+C,$$

and henceforth

$$\int_0^{2\pi}\frac{\sin^2\phi}{A^2(\phi)}\,\mathrm{d}\phi = 4\int_0^{\frac{\pi}{2}}\frac{\sin^2\phi}{A^2(\phi)}\,\mathrm{d}\phi = \frac{2}{\sqrt{\nu_1\nu_2}\nu_2}\arctan\left(\sqrt{\frac{\nu_2}{\nu_1}}\tan\phi\right)\Big|_0^{\frac{\pi}{2}} = \frac{\pi}{\sqrt{\nu_1\nu_2}\nu_2}.$$

Similarly,

$$\int \frac{\cos^2\phi}{A^2(\phi)}\,\mathrm{d}\phi = \int \frac{\sec^2\phi}{(\nu_1+\nu_2\tan^2\phi)^2}\,\mathrm{d}\phi = \frac{1}{\nu_1\sqrt{\nu_1\nu_2}} \underbrace{\int \frac{1}{\left[1+\left(\sqrt{\frac{\nu_2}{\nu_1}}\tan\phi\right)^2\right]^2}\,\mathrm{d}\left(\sqrt{\frac{\nu_2}{\nu_1}}\tan\phi\right)}_{I_1}$$

$$= \frac{1}{2\sqrt{\nu_1\nu_2}\nu_1}\arctan\left(\sqrt{\frac{\nu_2}{\nu_1}}\tan\phi\right) + \frac{1}{2\nu_1}\frac{\cos\phi\sin\phi}{\nu_1\cos^2\phi+\nu_2\sin^2\phi} + C.$$

Hence,

$$\int_0^{2\pi}\frac{\cos^2\phi}{A^2(\phi)}\,\mathrm{d}\phi = 4\int_0^{\frac{\pi}{2}}\frac{\cos^2\phi}{A^2(\phi)}\,\mathrm{d}\phi = \frac{2}{\sqrt{\nu_1\nu_2}\nu_1}\arctan\left(\sqrt{\frac{\nu_2}{\nu_1}}\tan\phi\right)\Bigg|_0^{\frac{\pi}{2}} = \frac{\pi}{\sqrt{\nu_1\nu_2}\nu_1}.$$

□

By virtue of Lemmas 2.3, 2.4, and 2.5, we are ready to prove the lower bound (1.13) in Theorem 1.1.

Proof of (1.13)

Let $\delta_0 > 0$ be the minimum threshold from the previous lemmas. By (2.15), (2.16), Lemma 2.4, and Lemma 2.5 we have

$$\varepsilon = \frac{\int_{\mathbb{S}^2} x^2\exp(-\nu_1x^2-\nu_2y^2)\,\mathrm{d}S}{\int_{\mathbb{S}^2}\exp(-\nu_1x^2-\nu_2y^2)\,\mathrm{d}S} \le \frac{\frac{\pi^4}{16}\int_0^{2\pi}\frac{\cos^2\phi}{A^2(\phi)}\,\mathrm{d}\phi}{\frac{1}{\pi}\int_0^{2\pi}\frac{1}{A(\phi)}\,\mathrm{d}\phi} = \frac{\pi^5}{32}\frac{1}{\nu_1}, \tag{2.35}$$

$$\varepsilon = \frac{\int_{\mathbb{S}^2} x^2\exp(-\nu_1x^2-\nu_2y^2)\,\mathrm{d}S}{\int_{\mathbb{S}^2}\exp(-\nu_1x^2-\nu_2y^2)\,\mathrm{d}S} \ge \frac{\frac{4}{\pi^3}\int_0^{2\pi}\frac{\cos^2\phi}{A^2(\phi)}\,\mathrm{d}\phi}{\frac{\pi^2}{4}\int_0^{2\pi}\frac{1}{A(\phi)}\,\mathrm{d}\phi} = \frac{8}{\pi^5}\frac{1}{\nu_1}, \tag{2.36}$$

$$\delta = \frac{\int_{\mathbb{S}^2} y^2\exp(-\nu_1x^2-\nu_2y^2)\,\mathrm{d}S}{\int_{\mathbb{S}^2}\exp(-\nu_1x^2-\nu_2y^2)\,\mathrm{d}S} \le \frac{\frac{\pi^4}{16}\int_0^{2\pi}\frac{\sin^2\phi}{A^2(\phi)}\,\mathrm{d}\phi}{\frac{1}{\pi}\int_0^{2\pi}\frac{1}{A(\phi)}\,\mathrm{d}\phi} = \frac{\pi^5}{32}\frac{1}{\nu_2}, \tag{2.37}$$

$$\delta = \frac{\int_{\mathbb{S}^2} y^2\exp(-\nu_1x^2-\nu_2y^2)\,\mathrm{d}S}{\int_{\mathbb{S}^2}\exp(-\nu_1x^2-\nu_2y^2)\,\mathrm{d}S} \ge \frac{\frac{4}{\pi^3}\int_0^{2\pi}\frac{\sin^2\phi}{A^2(\phi)}\,\mathrm{d}\phi}{\frac{\pi^2}{4}\int_0^{2\pi}\frac{1}{A(\phi)}\,\mathrm{d}\phi} = \frac{8}{\pi^5}\frac{1}{\nu_2}. \tag{2.38}$$

These estimates (2.35)-(2.38) together with (2.2), (2.17), Lemma 2.4, and Lemma 2.5 yield

$$f(Q) = -\ln Z + \sum_{i=1}^3 \mu_i\big(\lambda_i+\frac{1}{3}\big) = -\ln Z + \varepsilon\mu_1 + \delta\mu_2 + (1-\varepsilon-\delta)(-\mu_1-\mu_2)$$

$$= -\ln Z - \varepsilon\nu_1 - \delta\nu_2 - (\mu_1+\mu_2)$$

$$= -\ln\left[\int_{\mathbb{S}^2}\exp(\mu_1+\mu_2)\exp(\mu_1x^2+\mu_2y^2+\mu_3z^2)\,\mathrm{d}S\right] - \varepsilon\nu_1 - \delta\nu_2$$

$$
\begin{aligned}
&= -\ln \int_{\mathbb{S}^2} \exp(-\nu_1 x^2 - \nu_2 y^2)\, \mathrm{d}S - \varepsilon\nu_1 - \delta\nu_2 \geq -\ln\left[\frac{\pi^2}{4}\int_0^{2\pi} \frac{1}{A(\phi)}\, \mathrm{d}\phi\right] \\
&\quad - \varepsilon\nu_1 - \delta\nu_2 \\
&\geq \frac{1}{2}\ln(\nu_1\nu_2) - \ln 2\pi - \ln\frac{\pi^2}{4} - \frac{\pi^5}{16} \\
&\geq -\frac{1}{2}\ln(\varepsilon\delta) + \ln 16 - 8\ln\pi - \frac{\pi^5}{16}, \qquad \forall\, \delta < \delta_0,
\end{aligned} \tag{2.39}
$$

concluding the proof of (1.13).

Remark 2.3 Actually, (2.39) also provides a proof of the upper bound of the order

$$
C - \frac{1}{2}\ln\left(\lambda_1(Q) + \frac{1}{3}\right) - \frac{1}{2}\ln\left(\lambda_2(Q) + \frac{1}{3}\right)
$$

for an explicit constant C. However, it requires $\lambda_2(Q)$ to be sufficiently close to $-1/3$, which is not necessary in the argument regarding the upper bound of f provided in the previous subsection.

3 Blowup Rate of $\nabla_{\mathbb{Q}} f$

In this section, we shall finish the proof of Theorem 1.2, which plays a crucial role in the proofs regarding regularity results of the relevant solutions in both static and dynamic configurations (Evans et al. 2016; Geng and Tong 2020; Lu et al. 2020). The argument in the proof of (1.13) is no longer valid here in that now we only assume $\lambda_1(Q)$ is sufficiently close to $-1/3$.

To this end, we shall compute all five components of $\nabla_{\mathbb{Q}} f(Q)$, and state that only the "radial" and "tangential" components of $\nabla_{\mathbb{Q}} f$ are nonzero. Then we will be focused on the estimate of its "radial" component only.

Lemma 3.1 *For any physical Q-tensor of form* (2.1)*, it holds*

$$
\nabla_{rad} f(Q) = \sqrt{\frac{2}{3}} \frac{\mathrm{d} f(Q_\varepsilon^\perp)}{\mathrm{d}\varepsilon}\bigg|_{\varepsilon=0} = -\sqrt{\frac{3}{2}}\mu_1, \tag{3.1}
$$

$$
\nabla_{tan} f(Q) = \sqrt{\frac{1}{2}} \frac{\mathrm{d} f(Q_\varepsilon^\parallel)}{\mathrm{d}\varepsilon}\bigg|_{\varepsilon=0} = \sqrt{\frac{1}{2}}(\mu_1 + 2\mu_2). \tag{3.2}
$$

Here $\nabla_{rad} f(Q)$ (resp. $\nabla_{tan} f(Q)$) is defined in (3.3) *(resp. in* (3.4)*) as follows.*

Proof Recall from Geng and Tong (2020, Lemma C.1) that for a given physical Q-tensor of form (2.1), its projection on the physical boundary is

$$
Q^\perp = \begin{pmatrix} -\frac{1}{3} & 0 & 0 \\ 0 & \lambda_2 + \frac{\lambda_1 + \frac{1}{3}}{2} & 0 \\ 0 & 0 & \lambda_3 + \frac{\lambda_1 + \frac{1}{3}}{2} \end{pmatrix},
$$

and their distance is

$$d(Q) \stackrel{\text{def}}{=} |Q - Q^{\perp}| = \frac{\sqrt{6}}{2}\big(\lambda_1 + \frac{1}{3}\big).$$

Let us introduce

$$Q_\varepsilon^{(1)} \stackrel{\text{def}}{=} \begin{pmatrix} \lambda_1 - \varepsilon & 0 & 0 \\ 0 & \lambda_2 + \frac{\varepsilon}{2} & 0 \\ 0 & 0 & \lambda_3 + \frac{\varepsilon}{2} \end{pmatrix}, \qquad Q_\varepsilon^{(2)} \stackrel{\text{def}}{=} \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 + \varepsilon & 0 \\ 0 & 0 & \lambda_3 - \varepsilon \end{pmatrix},$$
$$Q_\varepsilon^{(3)} \stackrel{\text{def}}{=} \begin{pmatrix} \lambda_1 & \varepsilon & 0 \\ \varepsilon & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}, \qquad Q_\varepsilon^{(4)} \stackrel{\text{def}}{=} \begin{pmatrix} \lambda_1 & 0 & \varepsilon \\ 0 & \lambda_2 & 0 \\ \varepsilon & 0 & \lambda_3 \end{pmatrix}, \qquad Q_\varepsilon^{(5)} \stackrel{\text{def}}{=} \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & \varepsilon \\ 0 & \varepsilon & \lambda_3 \end{pmatrix}.$$

And for the sake of convenience, we refer to $Q_\varepsilon^{(1)} - Q$ (resp. $Q_\varepsilon^{(2)} - Q$) as the radial direction (resp. tangential direction). Note that these five directions $Q_\varepsilon^{(i)} - Q$, $1 \le i \le 5$ are orthogonal to one another in the sense that their inner product

$$\big(Q_\varepsilon^{(i)} - Q\big) : \big(Q_\varepsilon^{(j)} - Q\big) = 0, \qquad 1 \le i \ne j \le 5.$$

Step 1: radial component. We first calculate

$$\nabla_{rad} f(Q) \stackrel{\text{def}}{=} \lim_{\varepsilon \to 0} \frac{f(Q_\varepsilon^{(1)}) - f(Q)}{|Q_\varepsilon^{(1)} - Q|} = \sqrt{\frac{2}{3}} \frac{\mathrm{d} f(Q_\varepsilon^{(1)})}{\mathrm{d}\varepsilon}\bigg|_{\varepsilon=0}. \tag{3.3}$$

Let us denote $\rho_\varepsilon^{(1)}$ the associated Boltzmann distribution function of $f(Q_\varepsilon^{(1)})$:

$$\begin{aligned} \rho_\varepsilon^{(1)} &= \frac{\exp\big\{\mu_1^{(1)}(\varepsilon)x^2 + \mu_2^{(1)}(\varepsilon)y^2 + \mu_3^{(1)}(\varepsilon)z^2\big\}}{Z_\varepsilon^{(1)}}, \quad (x, y, z) \in \mathbb{S}^2, \\ Z_\varepsilon^{(1)} &= \int_{\mathbb{S}^2} \exp\big\{\mu_1^{(1)}(\varepsilon)x^2 + \mu_2^{(1)}(\varepsilon)y^2 + \mu_3^{(1)}(\varepsilon)z^2\big\}\,\mathrm{d}S, \\ &\quad \mu_1^{(1)}(\varepsilon) + \mu_2^{(1)}(\varepsilon) + \mu_3^{(1)}(\varepsilon) = 0, \\ \frac{1}{Z_\varepsilon^{(1)}} \frac{\partial Z_\varepsilon^{(1)}}{\partial \mu_i^{(1)}} &= \lambda_i^{(1)}(\varepsilon) + \frac{1}{3}, \qquad 1 \le i \le 3. \end{aligned}$$

Here $\lambda_i^{(1)}(\varepsilon)'s$, $1 \le i \le 3$ are eigenvalues of $Q_\varepsilon^{(1)}$. Clearly, ρ_0 (resp. μ_i, i = 1, 2, 3) is the optimal Boltzmann distribution (2.2) (resp. Lagrange multipliers) associated with Q. Note that

$$\lambda_1^{(1)}(\varepsilon) = \lambda_1 - \varepsilon, \quad \lambda_2^{(1)}(\varepsilon) = \lambda_2 + \frac{\varepsilon}{2}, \quad \lambda_3^{(1)}(\varepsilon) = \lambda_3 + \frac{\varepsilon}{2}.$$

As a consequence, direct computations give

$$\begin{aligned}
\frac{\mathrm{d}f(Q_\varepsilon^{(1)})}{\mathrm{d}\varepsilon} &= -\frac{\mathrm{d}\ln Z_\varepsilon^{(1)}}{\mathrm{d}\varepsilon} + \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\sum_{i=1}^{3}\mu_i^{(1)}(\varepsilon)\Big[\lambda_i^{(1)}(\varepsilon)+\frac{1}{3}\Big] \\
&= \underbrace{-\frac{\partial \ln Z_\varepsilon^{(1)}}{\partial\mu_i^{(1)}(\varepsilon)}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\mu_i^{(1)}(\varepsilon) + \sum_{i=1}^{3}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\mu_i^{(1)}(\varepsilon)\Big[\lambda_i^{(1)}(\varepsilon)+\frac{1}{3}\Big]}_{=0} + \sum_{i=1}^{3}\mu_i^{(1)}(\varepsilon)\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\lambda_i^{(1)}(\varepsilon) \\
&= -\mu_1^{(1)}(\varepsilon) + \frac{\mu_2^{(1)}(\varepsilon)+\mu_3^{(1)}(\varepsilon)}{2},
\end{aligned}$$

which gives (3.1) after evaluating at $\varepsilon = 0$.

Step 2: tangential component. We proceed to calculate

$$\nabla_{tan} f(Q) \stackrel{\text{def}}{=} \lim_{\varepsilon\to 0}\frac{f(Q_\varepsilon^{(2)}) - f(Q)}{\left|Q_\varepsilon^{(2)} - Q\right|} = \sqrt{\frac{2}{3}}\frac{\mathrm{d}f(Q_\varepsilon^{(2)})}{\mathrm{d}\varepsilon}\bigg|_{\varepsilon=0}. \tag{3.4}$$

Analogously, we denote $\rho_\varepsilon^{(2)}$ the associated Boltzmann distribution function of $f(Q_\varepsilon^{(2)})$:

$$\begin{aligned}
\rho_\varepsilon^{(2)} &= \frac{\exp\left\{\mu_1^{(2)}(\varepsilon)x^2 + \mu_2^{(2)}(\varepsilon)y^2 + \mu_3^{(2)}(\varepsilon)z^2\right\}}{Z_\varepsilon^{(2)}}, \quad (x,y,z)\in\mathbb{S}^2, \\
Z_\varepsilon^{(2)} &= \int_{\mathbb{S}^2}\exp\left\{\mu_1^{(2)}(\varepsilon)x^2 + \mu_2^{(2)}(\varepsilon)y^2 + \mu_3^{(2)}(\varepsilon)z^2\right\}\mathrm{d}S, \\
&\quad \mu_1^{(2)}(\varepsilon) + \mu_2^{(2)}(\varepsilon) + \mu_3^{(2)}(\varepsilon) = 0, \\
\frac{1}{Z_\varepsilon^{(2)}}\frac{\partial Z_\varepsilon^{(2)}}{\partial\mu_i^{(2)}} &= \lambda_i^{(2)}(\varepsilon) + \frac{1}{3}, \qquad 1 \le i \le 3.
\end{aligned}$$

Here $\lambda_i^{(2)}(\varepsilon)'s$, $1 \le i \le 3$ are eigenvalues of $Q_\varepsilon^{(2)}$. Apparently ρ_0 (resp. μ_i, i = 1, 2, 3) is the optimal Boltzmann distribution (2.2) (resp. Lagrange multipliers) associated with Q. Note that

$$\lambda_1^{(2)}(\varepsilon) = \lambda_1, \quad \lambda_2^{(2)}(\varepsilon) = \lambda_2 + \varepsilon, \quad \lambda_3^{(2)}(\varepsilon) = \lambda_3 - \varepsilon.$$

Then direct computations give

$$\begin{aligned}
\frac{\mathrm{d}f(Q_\varepsilon^{(2)})}{\mathrm{d}\varepsilon} &= \underbrace{-\frac{\partial\ln Z_\varepsilon^{(2)}}{\partial\mu_i^{(2)}(\varepsilon)}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\mu_i^{(2)}(\varepsilon) + \sum_{i=1}^{3}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\mu_i^{(2)}(\varepsilon)\Big[\lambda_i^{(2)}(\varepsilon)+\frac{1}{3}\Big]}_{=0} \\
&\quad + \sum_{i=1}^{3}\mu_i^{(2)}(\varepsilon)\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\lambda_i^{(2)}(\varepsilon) = \mu_2^{(2)}(\varepsilon) - \mu_3^{(2)}(\varepsilon),
\end{aligned}$$

which leads to (3.2) after evaluating at $\varepsilon = 0$.
Step 3: other components. We show that all three other components are identically zero. We first calculate

$$\nabla_3 f(Q) \overset{\text{def}}{=} \lim_{\varepsilon\to 0} \frac{f(Q_\varepsilon^{(3)}) - f(Q)}{\left|Q_\varepsilon^{(3)} - Q\right|} = \frac{\sqrt{2}}{2}\frac{\mathrm{d} f(Q_\varepsilon^{(3)})}{\mathrm{d}\varepsilon}\bigg|_{\varepsilon=0}. \tag{3.5}$$

Analogously, we denote $\rho_\varepsilon^{(3)}$ the associated Boltzmann distribution function of $f(Q_\varepsilon^{(3)})$:

$$\begin{aligned}
\rho_\varepsilon^{(3)} &= \frac{\exp\left\{\mu_1^{(3)}(\varepsilon)x^2 + \mu_2^{(3)}(\varepsilon)y^2 + \mu_3^{(3)}(\varepsilon)z^2\right\}}{Z_\varepsilon^{(3)}}, \quad (x, y, z) \in \mathbb{S}^2,\\
Z_\varepsilon^{(3)} &= \int_{\mathbb{S}^2} \exp\left\{\mu_1^{(3)}(\varepsilon)x^2 + \mu_2^{(3)}(\varepsilon)y^2 + \mu_3^{(3)}(\varepsilon)z^2\right\} \mathrm{d}S,\\
&\mu_1^{(3)}(\varepsilon) + \mu_2^{(3)}(\varepsilon) + \mu_3^{(3)}(\varepsilon) = 0,\\
\frac{1}{Z_\varepsilon^{(3)}}\frac{\partial Z_\varepsilon^{(3)}}{\partial \mu_i^{(3)}} &= \lambda_i^{(3)}(\varepsilon) + \frac{1}{3}, \qquad 1 \le i \le 3.
\end{aligned}$$

Here $\lambda_i^{(3)}(\varepsilon)'s$, $1 \le i \le 3$ are eigenvalues of $Q_\varepsilon^{(3)}$. Once again, ρ_0 (resp. μ_i, i = 1, 2, 3) is the optimal Boltzmann distribution (2.2) (resp. Lagrange multipliers) associated with Q. Note that

$$\lambda_1^{(3)}(\varepsilon) = \frac{\lambda_1 + \lambda_2 - \sqrt{(\lambda_1-\lambda_2)^2 + \varepsilon^2}}{2}, \lambda_2^{(3)}(\varepsilon) = \frac{\lambda_1 + \lambda_2 + \sqrt{(\lambda_1-\lambda_2)^2 + \varepsilon^2}}{2}, \lambda_3^{(3)}(\varepsilon) = \lambda_3.$$

Then direct computations give

$$\begin{aligned}
\frac{\mathrm{d} f(Q_\varepsilon^{(3)})}{\mathrm{d}\varepsilon} &= \underbrace{-\frac{\partial \ln Z_\varepsilon^{(3)}}{\partial \mu_i^{(3)}(\varepsilon)}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\mu_i^{(3)}(\varepsilon) + \sum_{i=1}^{3}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\mu_i^{(3)}(\varepsilon)\Big[\lambda_i^{(3)}(\varepsilon) + \frac{1}{3}\Big]}_{=0} + \sum_{i=1}^{3}\mu_i^{(3)}(\varepsilon)\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\lambda_i^{(3)}(\varepsilon)\\
&= \mu_1^{(3)}(\varepsilon)\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\lambda_1^{(3)}(\varepsilon) + \mu_2^{(3)}(\varepsilon)\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\lambda_2^{(3)}(\varepsilon).
\end{aligned}$$

Case 1: $\lambda_1 \neq \lambda_2$. Then

$$\frac{\mathrm{d} f(Q_\varepsilon^{(3)})}{\mathrm{d}\varepsilon}\bigg|_{\varepsilon=0} = -\frac{\mu_1^{(3)}(\varepsilon)}{2}\frac{\varepsilon}{\sqrt{(\lambda_1-\lambda_2)^2+\varepsilon^2}}\bigg|_{\varepsilon=0} + \frac{\mu_2^{(3)}(\varepsilon)}{2}\frac{\varepsilon}{\sqrt{(\lambda_1-\lambda_2)^2+\varepsilon^2}}\bigg|_{\varepsilon=0} = 0$$

Case 2: $\lambda_1 = \lambda_2$. Then $\lambda_1^{(3)}(\varepsilon) = \lambda_1 - \varepsilon$, $\lambda_2^{(3)}(\varepsilon) = \lambda_1 + \varepsilon$, and correspondingly

$$\frac{\mathrm{d} f(Q_\varepsilon^{(3)})}{\mathrm{d}\varepsilon}\bigg|_{\varepsilon=0} = -\mu_1 + \mu_2 = 0,$$

due to 2.1 and the assumption $\lambda_1 = \lambda_2$. In a similar way we can show that the other two components are identically zero. Hence, $\nabla f(Q) - 1/3\,\mathrm{tr}(\nabla f)\mathbb{I}_3$ depends on $\nabla_{rad} f(Q)$ and $\nabla_{tan} f(Q)$ only. □

As an immediate consequence, we have

Corollary 3.1 *For any physical Q-tensor of form (2.1), it holds*

$$1 \le \frac{\left|\nabla_{\mathbb{Q}} f(Q)\right|}{|\nabla_{rad} f(Q)|} \le 2. \tag{3.6}$$

Proof It suffices to prove the upper bound. It follows directly from Lemma 3.1 that

$$\left|\nabla_{\mathbb{Q}} f(Q)\right|^2 = \left|\nabla_{rad} f(Q)\right|^2 + \left|\nabla_{tan} f(Q)\right|^2 = \frac{3}{2}\mu_1^2 + \frac{1}{2}(\mu_1 + 2\mu_2)^2.$$

By (2.2) and Lemma 2.1, it is easy to check

$$3\mu_1 \le \mu_1 + 2\mu_2 \le 0,$$

which implies

$$\left|\nabla_{\mathbb{Q}} f(Q)\right|^2 \le \frac{3}{2}\mu_1^2 + \frac{1}{2}(3\mu_1)^2 = 6\mu_1^2,$$

and further together with (3.1) yields

$$1 \le \frac{\left|\nabla_{\mathbb{Q}} f(Q)\right|^2}{|\nabla_{rad} f(Q)|^2} \le \frac{6\mu_1^2}{\frac{3}{2}\mu_1^2} = 4.$$

Remark 3.1 It follows from Lemma 3.1 and Corollary 3.1 that, to estimate the blowup rate of $|\nabla_{\mathbb{Q}} f(Q)|$ as $\lambda_1(Q) \to -1/3$, it suffices to estimate μ_1.

[Proof of Theorem 1.2] The proof of Theorem 1.2 consists of the following two propositions, which provides the upper bound and lower bound of $|\nabla_{\mathbb{Q}} f|$, respectively.

Proposition 3.1 *For any physical Q-tensor of form (2.1), there exists a small computable constant $\varepsilon_0 > 0$, such that*

$$\left|\nabla_{\mathbb{Q}} f(Q)\right| \ge \frac{C_1}{\lambda_1 + \frac{1}{3}}, \qquad \textit{provided } 0 < \lambda_1 + \frac{1}{3} < \varepsilon_0, \tag{3.7}$$

where C_1 is given in (1.16).

Proof To begin with, we see from Lemma 3.1 that

$$\left|\nabla_{\mathbb{Q}} f(Q)\right|^2 \ge \left|\nabla_{rad} f(Q)\right|^2 = \frac{3}{2}\mu_1^2, \tag{3.8}$$

where μ_1 is the Lagrange multiplier associated with the Boltzmann distribution function of $f(Q)$ given in (2.2). Hence, it remains to estimate μ_1 in terms of $\lambda_1(Q)+1/3$, as $\lambda_1(Q)$ approaches $-1/3$. From (2.15), (2.16) we see

$$\lambda_1(Q)+\frac{1}{3}=\frac{\int_{\mathbb{S}^2} x^2\exp(-\nu_1x^2-\nu_2y^2)\,\mathrm{d}S}{\int_{\mathbb{S}^2}\exp(-\nu_1x^2-\nu_2y^2)\,\mathrm{d}S}. \tag{3.9}$$

Here ν_1,ν_2 are given in (2.17). Recall that

$$\nu_1\gg 1,\quad \nu_2\geq 0. \tag{3.10}$$

Step 1: Estimating the numerator in (3.9)

Using the coordinate system

$$v(x,\theta)\overset{\text{def}}{=}(x,\sqrt{1-x^2}\cos\theta,\sqrt{1-x^2}\sin\theta),\quad 0\leq x\leq 1,\ 0\leq\theta\leq 2\pi, \tag{3.11}$$

whose surface element is given by $|\frac{\partial v}{\partial x}\times\frac{\partial v}{\partial\theta}|=1$, we get

$$\begin{aligned}\int_{\mathbb{S}^2} x^2\exp(-\nu_1x^2-\nu_2y^2)\,\mathrm{d}S&=2\int_{\mathbb{S}^2\cap\{x\geq 0\}} x^2\exp(-\nu_1x^2-\nu_2y^2)\,\mathrm{d}S\\&=2\int_0^1 x^2e^{-\nu_1x^2}\Big[\int_0^{2\pi} e^{-\nu_2(1-x^2)\cos^2\theta}\,\mathrm{d}\theta\Big]\,\mathrm{d}x.\end{aligned} \tag{3.12}$$

Note that the zeroth modified Bessel function of first kind (Olver et al. 2010) is represented by

$$\mathrm{I}_0(\xi)=\frac{1}{\pi}\int_0^{\pi}\exp(\xi\cos\theta)\,\mathrm{d}\theta=\sum_{m=0}^{+\infty}\frac{1}{(m!)^2}\Big(\frac{\xi}{2}\Big)^{2m}, \tag{3.13}$$

and $\mathrm{I}_0(\xi)=\mathrm{I}_0(-\xi)$, hence we have

$$\begin{aligned}&\int_0^{2\pi} e^{-\nu_2(1-x^2)\cos^2\theta}\,\mathrm{d}\theta=\exp\Big\{\frac{-\nu_2(1-x^2)}{2}\Big\}\int_0^{2\pi}\exp\Big\{\frac{-\nu_2(1-x^2)\cos(2\theta)}{2}\Big\}\,\mathrm{d}\theta\\&\overset{(\eta=2\theta)}{=}\exp\Big\{\frac{-\nu_2(1-x^2)}{2}\Big\}\int_0^{2\pi}\exp\Big\{\frac{-\nu_2(1-x^2)\cos(\eta)}{2}\Big\}\,\mathrm{d}\eta\\&=\exp\Big\{\frac{-\nu_2(1-x^2)}{2}\Big\}\Big[\int_0^{\pi}\exp\Big\{\frac{-\nu_2(1-x^2)\cos(\eta)}{2}\Big\}\,\mathrm{d}\eta+\int_0^{\pi}\exp\Big\{\frac{\nu_2(1-x^2)\cos(\eta)}{2}\Big\}\,\mathrm{d}\eta\Big]\\&=2\pi\exp\Big\{\frac{-\nu_2(1-x^2)}{2}\Big\}\mathrm{I}_0\Big[\frac{\nu_2(1-x^2)}{2}\Big].\end{aligned}$$

Inserting the above identity into (3.12), together with (3.10), we obtain

$$\begin{aligned}&\int_{\mathbb{S}^2} x^2 \exp(-\nu_1 x^2 - \nu_2 y^2)\,\mathrm{d}S \\ &= 4\pi \int_0^1 x^2 e^{-\nu_1 x^2} \exp\left\{\frac{-\nu_2(1-x^2)}{2}\right\} \mathrm{I}_0\left[\frac{\nu_2(1-x^2)}{2}\right] \mathrm{d}x \\ &\geq 4\pi \int_0^{\frac{1}{\sqrt{\nu_1}}} x^2 e^{-\nu_1 x^2} \exp\left\{\frac{-\nu_2(1-x^2)}{2}\right\} \mathrm{I}_0\left[\frac{\nu_2(1-x^2)}{2}\right] \mathrm{d}x \\ &\geq 4\pi e^{-1} \int_0^{\frac{1}{\sqrt{\nu_1}}} x^2 \exp\left\{\frac{-\nu_2(1-x^2)}{2}\right\} \mathrm{I}_0\left[\frac{\nu_2(1-x^2)}{2}\right] \mathrm{d}x \end{aligned} \tag{3.14}$$

Meanwhile, since (Olver et al. 2010)

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\left[e^{-\xi}\mathrm{I}_0(\xi)\right] = e^{-\xi}\left[\mathrm{I}_1(\xi) - \mathrm{I}_0(\xi)\right] = \frac{e^{-\xi}}{\pi}\int_0^{\pi} (\cos\theta - 1)\exp(\xi\cos\theta)\,\mathrm{d}\theta < 0,$$

the function $\xi \mapsto e^{-\xi}\mathrm{I}_0(\xi)$ is strictly decreasing. Correspondingly we have

$$x \mapsto \exp\left\{\frac{-\nu_2(1-x^2)}{2}\right\}\mathrm{I}_0\left[\frac{\nu_2(1-x^2)}{2}\right] \quad \text{is strictly increasing for } x \in [0, 1]. \tag{3.15}$$

By virtue of (3.15), we get

$$\inf_{x\in[0,1/\sqrt{\nu_1}]} \exp\left\{\frac{-\nu_2(1-x^2)}{2}\right\}\mathrm{I}_0\left[\frac{\nu_2(1-x^2)}{2}\right] = \exp\left(\frac{-\nu_2}{2}\right)\mathrm{I}_0\left(\frac{\nu_2}{2}\right),$$

which together with (3.14) implies

$$\begin{aligned}\int_{\mathbb{S}^2} x^2 \exp(-\nu_1 x^2 - \nu_2 y^2)\,\mathrm{d}S &\geq \frac{4\pi}{e}\exp\left(\frac{-\nu_2}{2}\right)\mathrm{I}_0\left(\frac{\nu_2}{2}\right)\int_0^{\frac{1}{\sqrt{\nu_1}}} x^2\,\mathrm{d}x \\ &= \frac{4\pi}{3e}\exp\left(\frac{-\nu_2}{2}\right)\mathrm{I}_0\left(\frac{\nu_2}{2}\right)\nu_1^{-\frac{3}{2}}. \end{aligned} \tag{3.16}$$

Step 2: Estimating the denominator in (3.9)

Similar to the last step, we have

$$\begin{aligned}\int_{\mathbb{S}^2} \exp(-\nu_1 x^2 - \nu_2 y^2)\,\mathrm{d}S &= 4\pi \int_0^1 e^{-\nu_1 x^2} \exp\left\{\frac{-\nu_2(1-x^2)}{2}\right\}\mathrm{I}_0\left[\frac{\nu_2(1-x^2)}{2}\right]\mathrm{d}x \\ = 4\pi \int_0^{\frac{1}{\sqrt{2}}} & e^{-\nu_1 x^2} \exp\left\{\frac{-\nu_2(1-x^2)}{2}\right\}\mathrm{I}_0\left[\frac{\nu_2(1-x^2)}{2}\right]\mathrm{d}x \\ + 4\pi \int_{\frac{1}{\sqrt{2}}}^1 & e^{-\nu_1 x^2} \exp\left\{\frac{-\nu_2(1-x^2)}{2}\right\}\mathrm{I}_0\left[\frac{\nu_2(1-x^2)}{2}\right]\mathrm{d}x \end{aligned} \tag{3.17}$$

Recall (3.15), then we see

$$\int_{\frac{1}{\sqrt{2}}}^{1} e^{-\nu_1 x^2} \exp\left\{\frac{-\nu_2(1-x^2)}{2}\right\} \mathrm{I}_0\left[\frac{\nu_2(1-x^2)}{2}\right] \mathrm{d}x \le \int_{\frac{1}{\sqrt{2}}}^{1} e^{-\frac{\nu_1}{2}} \,\mathrm{d}x = \frac{2-\sqrt{2}}{2} e^{-\frac{\nu_1}{2}},$$

$$\int_0^{\frac{1}{\sqrt{2}}} e^{-\nu_1 x^2} \exp\left\{\frac{-\nu_2(1-x^2)}{2}\right\} \mathrm{I}_0\left[\frac{\nu_2(1-x^2)}{2}\right] \mathrm{d}x \le \exp\left(\frac{-\nu_2}{4}\right) \mathrm{I}_0\left(\frac{\nu_2}{4}\right) \int_0^{\frac{1}{\sqrt{2}}} e^{-\nu_1 x^2} \,\mathrm{d}x$$
$$\le \exp\left(\frac{-\nu_2}{4}\right) \mathrm{I}_0\left(\frac{\nu_2}{4}\right) \int_0^{\infty} e^{-\nu_1 x^2} \,\mathrm{d}x = \exp\left(\frac{-\nu_2}{4}\right) \mathrm{I}_0\left(\frac{\nu_2}{4}\right) \sqrt{\frac{\pi}{4\nu_1}}$$

Since $\xi \mapsto e^{-\xi/4}\mathrm{I}_0(\xi/4)$ is decreasing, while $\xi \mapsto \mathrm{I}_0(\xi/4)$ is increasing for $\xi \ge 0$, and $\nu_2 \le \nu_1$, $\nu_1 \gg 1$, there exists a computable, universal constant A_0 such that

$$\frac{2-\sqrt{2}}{2} e^{-\frac{\nu_1}{2}} \le \exp\left(\frac{-\nu_1}{4}\right) \sqrt{\frac{\pi}{4\nu_1}} \le \exp\left(\frac{-\nu_1}{4}\right) \mathrm{I}_0\left(\frac{\nu_1}{4}\right) \sqrt{\frac{\pi}{4\nu_1}}$$
$$\le \exp\left(\frac{-\nu_2}{4}\right) \mathrm{I}_0\left(\frac{\nu_2}{4}\right) \sqrt{\frac{\pi}{4\nu_1}}, \quad \forall \nu_1 \ge A_0.$$

To sum up, we conclude

$$\int_{\mathbb{S}^2} \exp(-\nu_1 x^2 - \nu_2 y^2) \,\mathrm{d}S \le 4\pi \exp\left(\frac{-\nu_2}{4}\right) \mathrm{I}_0\left(\frac{\nu_2}{4}\right) \sqrt{\frac{\pi}{\nu_1}}, \qquad \forall \nu_1 \ge A_0. \quad (3.18)$$

Step 3: Combining both estimates in (3.9)

We get immediately from (3.16) and (3.18) that

$$\lambda_1(Q) + \frac{1}{3} = \frac{1}{3e\sqrt{\pi}\nu_1} \frac{\exp\left(\frac{-\nu_2}{2}\right)\mathrm{I}_0\left(\frac{\nu_2}{2}\right)}{\exp\left(\frac{-\nu_2}{4}\right)\mathrm{I}_0\left(\frac{\nu_2}{4}\right)}, \qquad \forall \nu_1 \ge A_0. \quad (3.19)$$

Since $-3\mu_1 \ge \nu_1 \ge -\frac{3}{2}\mu_1$, it remains to bound the last fraction in (3.19). Since $e^{-\xi}\mathrm{I}_0(\xi) > 0$, $\forall \xi \ge 0$, and is equal to 1 at $\xi = 0$, it suffices to show

$$\liminf_{\xi \to +\infty} \frac{e^{-\xi}\mathrm{I}_0(\xi)}{e^{\frac{-\xi}{2}}\mathrm{I}_0(\frac{\xi}{2})} > 0 \quad (3.20)$$

The Taylor expansion of $e^{-\xi}\mathrm{I}_0(\xi)$, for $\xi \gg 1$, is (Olver et al. 2010)

$$e^{-\xi}\mathrm{I}_0(\xi) = \frac{1}{\sqrt{2\pi}}\left[\xi^{-\frac{1}{2}} + \frac{1}{8}\xi^{-\frac{3}{2}} + \frac{9}{128}\xi^{-\frac{5}{2}} + O(\xi^{-\frac{7}{2}})\right],$$

hence the limit in (3.20) is equal to $1/\sqrt{2}$. Thus, one can establish from (3.19) and the fact $-3\mu_1 \ge \nu_1 \ge -\frac{3}{2}\mu_1$ that

$$\lambda_1(Q) + \frac{1}{3} \ge \frac{1}{\nu_1} \frac{1}{3e\sqrt{\pi}} \inf_{\xi \ge 0} \frac{e^{-\xi}\mathrm{I}_0(\xi)}{e^{\frac{-\xi}{2}}\mathrm{I}_0(\frac{\xi}{2})}, \qquad \forall \nu_1 \ge A_0,$$

which further gives

$$\lambda_1(Q) + \frac{1}{3} \geq -\frac{1}{\mu_1}\frac{1}{9e\sqrt{\pi}} \inf_{\xi \geq 0} \frac{e^{-\xi} \mathrm{I}_0(\xi)}{e^{\frac{-\xi}{2}} \mathrm{I}_0(\frac{\xi}{2})}, \quad \text{provided } \mu_1 < -\frac{2A_0}{3}. \tag{3.21}$$

In view of Remark 2.1, there exists a small computable constant $\varepsilon_0 > 0$, such that

$$\mu_1 < -\frac{2A_0}{3}, \quad \text{provided } 0 < \lambda_1(Q) + \frac{1}{3} < \varepsilon_0.$$

In all, using (1.16) we conclude that from (3.21) that

$$\left|\nabla_{\mathbb{Q}} f(Q)\right| \geq \left|\nabla_{rad} f(Q)\right| \geq \frac{\sqrt{6}}{2}\mu_1 \geq \frac{C_1}{\lambda_1(Q) + \frac{1}{3}}, \quad \text{provided}$$
$$0 < \lambda_1(Q) + \frac{1}{3} < \varepsilon_0, \tag{3.22}$$

completing the proof. □

Proposition 3.2 *For any physical Q-tensor of form (2.1), there exists a small computable constant $\varepsilon_0 > 0$, such that*

$$\left|\nabla_{\mathbb{Q}} f(Q)\right| \leq \frac{C_2}{\lambda_1 + \frac{1}{3}}, \qquad \textit{provided } 0 < \lambda_1 + \frac{1}{3} < \varepsilon_0, \tag{3.23}$$

where C_2 is given in (1.16).

Proof In contrast to the proof of Proposition 3.1, we need to obtain suitable upper bound on the numerator of (3.9), but lower bound on the denominator of (3.9).

Step 1: Estimating the numerator in (3.9)

Using the coordinate system (3.11), similar to the proof of Proposition 3.1 one can establish

$$\begin{aligned}\int_{\mathbb{S}^2} x^2 \exp(-\nu_1 x^2 - \nu_2 y^2)\,\mathrm{d}S &= 4\pi \int_0^1 x^2 e^{-\nu_1 x^2} \exp\left\{\frac{-\nu_2(1-x^2)}{2}\right\} \mathrm{I}_0\left[\frac{\nu_2(1-x^2)}{2}\right] \mathrm{d}x \\ &= 4\pi \int_0^{\frac{1}{\sqrt{2}}} x^2 e^{-\nu_1 x^2} \exp\left\{\frac{-\nu_2(1-x^2)}{2}\right\} \mathrm{I}_0\left[\frac{\nu_2(1-x^2)}{2}\right] \mathrm{d}x \\ &\quad + 4\pi \int_{\frac{1}{\sqrt{2}}}^1 x^2 e^{-\nu_1 x^2} \exp\left\{\frac{-\nu_2(1-x^2)}{2}\right\} \mathrm{I}_0\left[\frac{\nu_2(1-x^2)}{2}\right] \mathrm{d}x, \\ &\doteq 4\pi(J_1 + J_2).\end{aligned} \tag{3.24}$$

In view of (3.15), we get

$$J_2 \leq \int_{\frac{1}{\sqrt{2}}}^1 x^2 e^{-\nu_1 x^2}\,\mathrm{d}x = \frac{2-\sqrt{2}}{2} e^{-\frac{\nu_1}{2}}, \tag{3.25}$$

and

$$
\begin{aligned}
J_1 &\le \int_0^{\frac{1}{\sqrt{2}}} x^2 e^{-\nu_1 x^2} \exp\Big(-\frac{\nu_2}{4}\Big)\mathrm{I}_0\Big(\frac{\nu_2}{4}\Big)\,\mathrm{d}x \\
&= \exp\Big(-\frac{\nu_2}{4}\Big)\mathrm{I}_0\Big(\frac{\nu_2}{4}\Big)\left[-\frac{e^{-\frac{\nu_1}{2}}}{2\sqrt{2}\nu_1}+\frac{1}{2\nu_1}\int_0^{\frac{1}{\sqrt{2}}} e^{-\nu_1 x^2}\,\mathrm{d}x\right] \\
&\le \exp\Big(-\frac{\nu_2}{4}\Big)\mathrm{I}_0\Big(\frac{\nu_2}{4}\Big)\Big[-\frac{e^{-\frac{\nu_1}{2}}}{2\sqrt{2}\nu_1}+\frac{1}{2\nu_1}\int_0^{+\infty} e^{-\nu_1 x^2}\,\mathrm{d}x\Big] \\
&= \exp\Big(-\frac{\nu_2}{4}\Big)\mathrm{I}_0\Big(\frac{\nu_2}{4}\Big)\Big[-\frac{e^{-\frac{\nu_1}{2}}}{2\sqrt{2}\nu_1}+\frac{\sqrt{\pi}}{4}\nu_1^{-\frac{3}{2}}\Big].
\end{aligned}
\tag{3.26}
$$

Since $\nu_2 \le \nu_1$, and $\xi \mapsto e^{-\xi}\mathrm{I}_0(\xi)$ is decreasing, we have

$$
\begin{aligned}
0 &< \frac{e^{-\frac{\nu_1}{2}}}{\exp\big(-\frac{\nu_2}{4}\big)\mathrm{I}_0\big(\frac{\nu_2}{4}\big)\sqrt{\pi}/4\nu_1^{\frac{3}{2}}} \le \frac{e^{-\frac{\nu_1}{2}}}{\exp\big(-\frac{\nu_1}{4}\big)\mathrm{I}_0\big(\frac{\nu_1}{4}\big)\sqrt{\pi}/4\nu_1^{\frac{3}{2}}} \\
&= \frac{4\nu_1^{\frac{3}{2}}}{e^{\frac{\nu_1}{4}}\mathrm{I}_0\big(\frac{\nu_1}{4}\big)\sqrt{\pi}} \longrightarrow 0, \quad \text{as} \quad \nu_1 \to +\infty.
\end{aligned}
$$

Hence, there exists a computable constant $A_0 > 0$, such that

$$
\begin{aligned}
J_1 + J_2 &\le \frac{2-\sqrt{2}}{2}e^{-\frac{\nu_1}{2}} + \exp\Big(-\frac{\nu_2}{4}\Big)\mathrm{I}_0\Big(\frac{\nu_2}{4}\Big)\Big[-\frac{e^{-\frac{\nu_1}{2}}}{2\sqrt{2}\nu_1}+\frac{\sqrt{\pi}}{4}\nu_1^{-\frac{3}{2}}\Big] \\
&\le 4\pi\exp\Big(-\frac{\nu_2}{4}\Big)\mathrm{I}_0\Big(\frac{\nu_2}{4}\Big)\sqrt{\pi}\,\nu_1^{-\frac{3}{2}}, \quad \forall \nu_1 > A_0,
\end{aligned}
$$

which inserts into (3.24) yields

$$
\begin{aligned}
&\int_{\mathbb{S}^2} x^2 \exp(-\nu_1 x^2 - \nu_2 y^2)\,\mathrm{d}S \le 4\pi(J_1 + J_2) \le 4\pi \\
&\quad \le \exp\Big(-\frac{\nu_2}{4}\Big)\mathrm{I}_0\Big(\frac{\nu_2}{4}\Big)\sqrt{\pi}\,\nu_1^{-\frac{3}{2}}, \quad \forall \nu_1 > A_0.
\end{aligned}
\tag{3.27}
$$

Step 2: Estimating the denominator in (3.9)

Using (3.10), the coordinate system (3.11) and (3.15), we get

$$
\begin{aligned}
\int_{\mathbb{S}^2} \exp(-\nu_1 x^2 - \nu_2 y^2)\,\mathrm{d}S &= 4\pi\int_0^1 e^{-\nu_1 x^2}\exp\Big\{\frac{-\nu_2(1-x^2)}{2}\Big\}\mathrm{I}_0\Big[\frac{\nu_2(1-x^2)}{2}\Big]\,\mathrm{d}x \\
&\ge 4\pi\int_0^{\frac{1}{\sqrt{\nu_1}}} e^{-\nu_1 x^2}\exp\Big\{\frac{-\nu_2(1-x^2)}{2}\Big\}\mathrm{I}_0\Big[\frac{\nu_2(1-x^2)}{2}\Big]\,\mathrm{d}x \\
&\ge \frac{4\pi}{e\sqrt{\nu_1}}\exp\Big[-\frac{\nu_2}{2}\Big]\mathrm{I}_0\Big(\frac{\nu_2}{2}\Big)
\end{aligned}
\tag{3.28}
$$

Step 3: Completing the proof

Combining (3.27) and (3.28), we see that

$$\lambda_1(Q)+\frac{1}{3}\leq\frac{\exp\big(-\frac{\nu_2}{4}\big)\mathrm{I}_0\big(\frac{\nu_2}{4}\big)\sqrt{\pi}\nu_1^{-\frac{3}{2}}}{\frac{1}{e\sqrt{\nu_1}}\exp\big(-\frac{\nu_2}{2}\big)\mathrm{I}_0\big(\frac{\nu_2}{2}\big)}\leq\frac{e\sqrt{\pi}}{\nu_1}\sup_{\xi\geq 0}\frac{\exp\big(-\frac{\xi}{4}\big)\mathrm{I}_0\big(\frac{\xi}{4}\big)}{\exp\big(-\frac{\xi}{2}\big)\mathrm{I}_0\big(\frac{\xi}{2}\big)},\qquad\forall\nu_1>A_0\quad(3.29)$$

where

$$\sup_{\xi\geq 0}\frac{\exp\big(-\frac{\xi}{4}\big)\mathrm{I}_0\big(\frac{\xi}{4}\big)}{\exp\big(-\frac{\xi}{2}\big)\mathrm{I}_0\big(\frac{\xi}{2}\big)}\geq\frac{\mathrm{I}_0(0)}{\mathrm{I}_0(0)}=1.$$

Therefore, together with the fact that $\mu_1\leq\mu_2\leq-\mu_1/2$, we know

$$-\mu_1\leq-2\mu_1-\mu_2=\nu_1\leq\frac{1}{\lambda_1(Q)+\frac{1}{3}}e\sqrt{\pi}\sup_{\xi\geq 0}\frac{\exp\big(-\frac{\xi}{4}\big)\mathrm{I}_0\big(\frac{\xi}{4}\big)}{\exp\big(-\frac{\xi}{2}\big)\mathrm{I}_0\big(\frac{\xi}{2}\big)},\qquad\forall\nu_1>A_0.$$

Then following the same argument in the proof of Proposition 3.2, we conclude from Corollary 3.1 that as $\lambda_1(Q)\to-1/3$, it holds

$$\big|\nabla_{\mathbb{Q}}f(Q)\big|\leq 2|\nabla_{rad}f(Q)|=-\sqrt{6}\mu_1=\frac{C_2}{\lambda_1(Q)+\frac{1}{3}},\qquad(3.30)$$

where C_2 is given in Theorem 1.16, completing the proof. □

Remark 3.2 Using similar argument, it is expected that the estimate for second-order derivatives of f near its physical boundary could be achieved.

Acknowledgements We would like to thank Professor John Ball for his kind discussions, especially pointing out several useful references to us. We thank the anonymous referees for their suggestions to improve the quality of our paper. X. Y. Lu's work is supported by his NSERC Discovery Grant "Regularity of minimizers and pattern formation in geometric minimization problems." X. Xu's work is supported by the NSF Grant DMS-2007157 and the Simons Foundation Grant No. 635288. W. J. Zhang's work is supported by NSF Grant DMS-1818861.

References

Ball, J.: Mathematics of liquid crystals. Cambridge Centre for Analysis short course, 13–17 (2012)

Ball, J.: Analysis of liquid crystals and their defects, Lecture notes of the Scuola Estiva GNFM, Ravello, 17–22 (2018)

Ball, J., Majumdar, A.: Nematic liquid crystals: from Maier-Saupe to a continuum theory. Mol. Cryst. Liq. Cryst. **525**, 1–11 (2010)

Ball, J., Majumdar, A.: Passage from the mean-field Maier-Saupe to the continuum Landau-de Gennes theory for nematic liquid crystals, work in progress

Bauman, P., Phillips, D.: Regularity and the behavior of eigenvalues for minimizers of a constrained Q-tensor energy for liquid crystals. Calc. Var. Partial Differ. Equ. **55**, 55–81 (2016)

Berreman, D.W., Meiboom, S.: Tensor representation of Oseen-Frank strain energy in uniaxial cholesterics. Phys. Rev. A **30**, 1955–1959 (1984)

Davis, T.A., Gartland, E.C.: Finite element analysis of the Landau-de Gennes minimization problem for liquid crystals. SIAM J. Numer. Anal. **35**(1), 336–362 (1998)

de Gennes, P.G., Prost, J.: The Physics of Liquid Crystals. Oxford Science Publications, Oxford (1993)

Dickmann, S.: Numerische Berechnung von Feld und Molekülausrichtung in Flüssigkristallanzeigen. Ph.D. thesis, University of Karlsruhe (1995)

Du, H.R., Hu, X.P., Wang, C.Y.: Suitable weak solutions for the co-rotational Beris-Edwards system in dimension three. Arch. Ration. Mech. Anal. **238**(1), 749–803 (2020)

Evans, L.C., Kneuss, O., Tran, H.: Partial regularity for minimizers of singular energy functionals, with application to liquid crystal models. Trans. Am. Math. Soc. **368**(5), 3389–3413 (2016)

Feireisl, E., Rocca, E., Schimperna, G., Zarnescu, A.: Evolution of non-isothermal Landau-de Gennes nematic liquid crystals flows with singular potential. Commun. Math. Sci. **12**, 317–343 (2014)

Feireisl, E., Rocca, E., Schimperna, G., Zarnescu, A.: Nonisothermal nematic liquid crystal flows with the Ball-Majumdar free energy. Annali di Mat. Pura ed App. **194**(5), 1269–1299 (2015)

Geng, Z.Y., Tong, J.J.: Regularity of minimizers of a tensor-valued variational obstacle problem in three dimensions. Calc. Var. **59**, 57 (2020). https://doi.org/10.1007/s00526-020-1717-7

Golovaty, D., Kim, Y.K., Lavrentovich, O., Novack, M., Sternberg, P.: Phase transitions in nematics: textures with tactoids and disclinations. Math. Model. Nat. Phenom. **15**(8), 10 (2020a)

Golovaty, D., Novack, M., Sternberg, P.: A novel Landau-de Gennes model with quartic elastic terms. Eur. J. Appl. Math. **32**(1), 177–198 (2020b)

Katriel, L., Kventse, G.F., Luckhurst, G., Sluckin, T.: Free energies in the Landau and molecular field approaches. Mol. Cryst. Liquid Cryst. **1**, 337–355 (1986)

Kitavtsev, G., Robbins, J.M., Slastikov, V., Zarnescu, A.: Liquid crystal defects in the Landau-de Gennes theory in two dimensions-beyond the one-constant approximation. Math. Models Methods Appl. Sci. **26**(14), 2769–2808 (2016)

Iyer, G., Xu, X., Zarnescu, A.: Dynamic cubic instability in a 2D Q-tensor model for liquid crystals. Math. Models Methods Appl. Sci. **25**(8), 1477–1517 (2015)

Lu, X.Y., Liu, Y.N., Xu, X.: Regularity of a gradient flow generated by the anisotropic Landau-de Gennes energy with a singular potential. arXiv:2011.09541v2 (2020)

Longa, L., Monselesan, D., Trebin, H.R.: An extension of the Landau-Ginzburg-de Gennes theory for liquid crystals. Liq. Cryst. **2**(6), 769–796 (1987)

Maier, W., Saupe, A.: A simple molecular statistical theory of the nematic crystalline-liquid phase. I Z Naturf. a **14**, 882–889 (1959)

Majumdar, A.: Equilibrium order parameters of liquid crystals in the Landau-de Gennes theory. Eur. J. Appl. Math. **21**(2), 181–203 (2010)

Majumdar, A., Zarnescu, A.: Landau-De Gennes theory of nematic liquid crystals: the Oseen-Frank limit and beyond. Arch. Ration. Mech. Anal. **196**(1), 227–280 (2010)

Mottram, N.J., Newton, J.P.: Introduction to Q-tensor theory. arXiv preprint, arXiv:1409.3542 (2014)

Olver, F., Lozier, D., Boisvert, R., Clark, C.: NIST Handbook of Mathematical Functions. Cambridge University Press, Cambridge (2010)

Paicu, M., Zarnescu, A.: Global existence and regularity for the full coupled Navier–Stokes and Q-tensor system. SIAM J. Math. Anal. **43**(5), 2009–2049 (2011)

Paicu, M., Zarnescu, A.: Energy dissipation and regularity for a coupled Navier–Stokes and Q-tensor system. Arch. Ration. Mech. Anal. **203**(1), 45–67 (2012)

Virga, E.: Variational Theories for Liquid Crystals, Applied Mathematics and Mathematical Computation, 8. Chapman & Hall, London (1994)

Wilkinson, M.: Strict physicality of global weak solutions of a Navier–Stokes Q-tensor system with singular potential. Arch. Ration. Mech. Anal. **218**, 487–526 (2015)

Wu, H., Xu, X., Zarnescu, A.: Dynamics and flow effects in the Beris-Edwards system modelling nematic liquid crystals. Arch. Rational Mech. Anal. **231**, 1217–1267 (2019)