Blowup rate estimates of the Ball-Majumdar potential and its gradient in the Landau-de Gennes theory

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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 singular potential, called Ball-Majumdar potential, is introduced in [3], and 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.

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 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 \([6, 17, 24]\). Let \(n\) be a unit vector in \(\mathbb{R}^3\), representing the orientation of a single liquid crystal molecule and \(\rho(x; n)\) 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 \(\rho\) from its isotropic value, reads

\[ Q = \int_{S^2} [\rho(n) \otimes \rho(n) - \frac{1}{3} I_3] \, dn. \]  

(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 \(-1/3 \leq \lambda_i(Q) \leq 2/3, 1 \leq i \leq 3\).

In the continuum model, instead, a phenomenological Landau-de Gennes theory is proposed [1, 6, 20] such that the alignment of liquid crystal molecules is described by the macroscopic \(Q\)-tensor order parameter, which is a symmetric, traceless \(3 \times 3\) 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 [1,13]:

\[ \mathcal{E}[Q] = \int_{\Omega} \mathcal{F}(Q(x)) \, dx, \]  

(1.2)

where \(Q\) is the basic element in the so called \(Q\)-tensor space \(\mathbb{H}\)

\[ \mathbb{S}_0^{(3)} \overset{\text{def}}{=} \{ M \in \mathbb{R}^{3 \times 3} \mid \text{tr}(M) = 0, M^T = M \} \].

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 \(Q\) [19,22,23]

\[ \mathcal{F}_{bulk} = \frac{a}{2} \text{tr}(Q^2) + \frac{b}{3} \text{tr}(Q^3) + \frac{c}{4} r^2(Q^2), \]  

(1.3)

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where \( a, b, c \) are assumed to be material-dependent coefficients. While the simplest form of the elastic part \( F_{el} \) that is invariant under rigid rotations and material symmetry is \( 13, 16 \):

\[
F_{el} = L_1 |\nabla Q|^2 + L_2 \partial_i Q_{ik} \partial_k Q_{ij} + L_3 \partial_j Q_{ij} \partial_l Q_{ik} + L_4 Q_{ik} \partial_i Q_{kj} \partial_j Q_{ij}.
\] (1.4)

Here \( \partial_i Q_{ij} \) stands for the \( i \)-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 \( 14 \). On the other hand, however, this cubic term makes the elastic energy part \( F_{el} \) unbounded from below \( 3 \).

To overcome this issue, a singular bulk potential \( \psi_B \) is introduced in \( 3 \) to replace the regular potential \( F_{bulk} \). Specifically, the Ball-Majumdar potential \( f \) is defined by

\[
f(Q) \overset{\text{def}}{=} \begin{cases} 
\inf_{\rho \in A_Q} \int_{\mathbb{S}^2} \rho(n) \ln \rho(n) \, dn, & -\frac{1}{3} < \lambda_i(Q) < \frac{2}{3}, 1 \leq i \leq 3 \\
+\infty, & \text{otherwise},
\end{cases}
\] (1.5)

where the admissible set \( A_Q \) is

\[
A_Q = \left\{ \rho \in \mathcal{P}(\mathbb{S}^2), \rho(n) = \rho(-n), \int_{\mathbb{S}^2} [\rho(n) \otimes \rho(n) - \frac{1}{3} \mathbb{I}_3] \, dn = Q \right\}
\] (1.6)

In other words, we minimize the Boltzmann entropy over all probability distributions \( \rho \) with given normalized second moment \( Q \). Correspondingly,

\[
\psi_B(Q) = f(Q) - \frac{k}{2} |Q|^2
\] (1.7)

is used to replace the commonly employed bulk potential \( F_{bulk} \), where the last polynomial term is added to ensure the existence of local energy minimizers, and \( k > 0 \) is a constant. As a consequence, \( \psi_B \) imposes a natural enforcement of a physical constraint on the eigenvalues of the mathematical \( Q \)-tensor. Further, the elastic energy part \( F_{el} \) could be kept under control under mild assumptions on \( L_1, \cdots, L_4 \) \( 5, 13, 14 \). Interested readers may also see \( 12 \) 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 recent development. Concerning dynamic configurations, in a non-isothermal co-rotational Beris-Edwards system whose free energy consists of one elastic constant term and this singular potential, the existence of global in time weak solutions is established in \( 9, 10 \), and the convexity of \( f \) is proved in \( 10 \). The existence, regularity and strict physicality of global weak solutions of the corresponding isothermal co-rotational Beris-Edwards system is investigated in \( 26 \), while global existence and partial regularity of a suitable weak solution to this system is established in \( 7 \). The eigenvalue preservation of the co-rotational Beris-Edwards system with the regular bulk potential is studied in \( 26 \) by virtue of \( f \). Meanwhile, in static configurations, the Hölder regularity of energy minimizer in \( 2D \) is established in \( 4 \), while partial regularity results for the energy minimizer are given in \( 8 \), and further improved in \( 8 \) under various assumptions of the blowup rates of \( f \) and its gradient as \( Q \) approaches its physical boundary.

Motivated by all the existing work, especially the aforementioned study in static configurations, in this paper we revisit the Ball-Majumdar potential \( f \), and aim to establish the blowup rates of \( f \), as well as its gradient \( \nabla f \) near its physical boundary. In view of \( 13, 15 \), here and after we always assume \( Q \) is physical, in the sense that

\[
-\frac{1}{3} < \lambda_i(Q) < \frac{2}{3}, \quad 1 \leq i \leq 3.
\] (1.8)

First, using a constructive proof we can provide an alternative upper bound for the blowup rate of \( f(Q) \) as \( Q \) approaches its physical boundary, as illustrated in the next Theorem.

**Theorem 1.1.** For any physical \( Q \)-tensor, assume \( \lambda_1(Q) \leq \lambda_2(Q) \leq \lambda_3(Q) \). Then as \( \lambda_1(Q) \to -1/3 \), the functional \( f \) defined in \( 13, 15 \) is bounded above by

\[
f(Q) \leq -\ln 24 - \frac{1}{2} \ln \left( \lambda_1(Q) + \frac{1}{3} \right) - \frac{1}{2} \ln \left( \lambda_2(Q) + \frac{1}{3} \right).
\] (1.9)
Remark 1.1. We want to point out that this upper bound \([19]\), together with the following blowup rate\([2]\)

\[
\frac{1}{2} \ln \left(\frac{1}{(2\pi)^3 e(\lambda_1(Q) + \frac{1}{3})}\right) \leq f(Q) \leq \ln \left(\frac{1}{\lambda_1(Q) + \frac{1}{3}}\right),
\]

(1.10)
does provide extra information for the blowup behavior of \(f\), see Remark\([2] \) for details.

More importantly, the next theorem gives a blowup rate of \(\nabla f\) near the physical boundary of \(Q\). Throughout our paper for a matrix \(R \in \mathbb{R}^{3 \times 3}\), \(\|R\|_F = \sqrt{\text{tr}(R^TR)}\) stands for its Frobenius norm.

Theorem 1.2. For any physical \(Q\)-tensor, assume \(\lambda_1(Q) \leq \lambda_2(Q) \leq \lambda_3(Q)\). Then as \(\lambda_1(Q) \to -1/3\), the gradient of the functional \(f\) defined in \([1,3]\) satisfies

\[
\frac{C_1}{\lambda_1(Q) + \frac{1}{3}} \leq \|\nabla f(Q)\|_F \leq \frac{C_2}{\lambda_1(Q) + \frac{1}{3}},
\]

(1.11)

with the constants \(C_1\) and \(C_2\) given by

\[
C_1 = \sqrt{\frac{3}{2\pi e}} \cdot \inf_{\xi \geq 0} e^{-\xi} I_0(\xi) > 0, \quad C_2 = \sqrt{6\pi e} \cdot \sup_{\xi \geq 0} \exp \left( -\frac{\xi}{2} \right) I_0(\frac{\xi}{2}).
\]

(1.12)

Here \(I_0(\cdot)\) is the zeroth order modified Bessel function of first kind.

This paper is organized as follows. In Section 2, we present an alternative result regarding the upper bound in the blowup rate of \(f\). In Section 3, we give a proof of Theorem 1.2.

2 Blowup rate of \(f\)

Note that \([18]\) is equivalent to \(Q \in \mathcal{D}(f)\), namely the effective domain of \(f\) where \(f\) assumes finite values. As proved in \([9]\), \(f\) is smooth for \(Q \in \mathcal{D}(f)\). Since \(f\) is rotation invariant \([1]\), here and after, we always assume that any considered physical \(Q\)-tensor is diagonal:

\[
Q = \begin{pmatrix}
\lambda_1 & 0 & 0 \\
0 & \lambda_2 & 0 \\
0 & 0 & \lambda_3
\end{pmatrix}, \quad -\frac{1}{3} < \lambda_1 \leq \lambda_2 \leq \lambda_3 < \frac{2}{3}, \quad \lambda_1 + \lambda_2 + \lambda_3 = 0.
\]

(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 \(f(Q) = \int_{\mathbb{S}^2} \rho_Q \log \rho_Q \, dS\) is given by \([1,3]\)

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

(2.2)

with

\[
Z(\mu_1,\mu_2,\mu_3) = \int_{\mathbb{S}^2} \exp(\mu_1 x^2 + \mu_2 y^2 + \mu_3 z^2) \, dS.
\]

(2.3)

To begin with, we have

Lemma 2.1. For any physical \(Q\)-tensor \([2,3]\), its optimal probability density \(\rho_Q\) defined in \(2.2\) satisfies

\[
\mu_1 \leq \mu_2 \leq \mu_3.
\]

And \(\mu_i = \mu_j\) provided \(\lambda_i = \lambda_j\) for \(1 \leq i \neq j \leq 3\).

Proof. By symmetry, it suffices to prove that \(\mu_i\) is increasing in \(\lambda_i\), i.e. \(\mu_1 < \mu_2\) whenever \(\lambda_1 < \lambda_2\).

Consider eigenvalues \(\lambda_1 < \lambda_2\). Then it holds

\[
\int_{\mathbb{S}^2} x^2 \rho_Q \, dV = \lambda_1 + \frac{1}{3} < \lambda_2 + \frac{1}{3} = \int_{\mathbb{S}^2} y^2 \rho_Q \, dS
\]

(2.4)

From \(2.2\) we get

\[
\rho_Q = \frac{\exp \left\{ \mu_1 x^2 + \mu_2 y^2 - (\mu_1 + \mu_2)(1 - x^2 - y^2) \right\}}{\int_{\mathbb{S}^2} \exp(\mu_1 x^2 + \mu_2 y^2 - (\mu_1 + \mu_2)(1 - x^2 - y^2)) \, dS} = m^* \exp \left\{ (2\mu_1 + \mu_2)x^2 + (\mu_1 + 2\mu_2)y^2 \right\},
\]
where

\[ m^* = \frac{1}{\int_{S^2} \exp \{ (2\mu_1 + \mu_2)x^2 + (\mu_1 + 2\mu_2)y^2 \} \, dS} \]  

(2.5)

Assume, by contradiction, that \( \mu_1 \geq \mu_2 \). Using spherical coordinates

\[
\begin{cases}
  x = \sin \theta \cos \phi \\
  y = \sin \theta \sin \phi \\
  z = \cos \theta
\end{cases}
\]

we get from (2.4) that

\[
\lambda_1 - \lambda_2 = \int_{S^2} x^2 \rho_Q \, dS - \int_{S^2} y^2 \rho_Q \, dS
\]

\[
= 8m^* \int_0^\pi \int_0^{\pi/2} (\cos^2 \phi - \sin^2 \phi) \exp \{ (\mu_1 - \mu_2) \sin^2 \theta \cos^2 \phi \} \, d\phi \exp \{ (\mu_1 + 2\mu_2) \sin^2 \theta \} \sin^3 \theta \, d\theta
\]

\[
= 8m^* \left[ \int_0^\pi \int_0^{\pi/2} (\cos^2 \phi - \sin^2 \phi) \exp \{ (\mu_1 - \mu_2) \sin^2 \theta \cos^2 \phi \} \, d\phi \exp \{ (\mu_1 + 2\mu_2) \sin^2 \theta \} \sin^3 \theta \, d\theta \\
+ \int_\pi^{3\pi/2} \int_0^{\pi/2} (\cos^2 \phi - \sin^2 \phi) \exp \{ (\mu_1 - \mu_2) \sin^2 \theta \cos^2 \phi \} \, d\phi \exp \{ (\mu_1 + 2\mu_2) \sin^2 \theta \} \sin^3 \theta \, d\theta \right]
\]

\[
= 8m^* \int_0^\pi \int_0^{\pi/2} (\cos^2 \phi - \sin^2 \phi) \left( \exp \{ (\mu_1 - \mu_2) \sin^2 \theta \cos^2 \phi \} - \exp \{ (\mu_1 - \mu_2) \sin^2 \theta \sin^2 \phi \} \right) \, d\phi \exp \{ (\mu_1 + 2\mu_2) \sin^2 \theta \} \sin^3 \theta \, d\theta
\]

\[
\geq 0
\]

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 \( \mu_1 \) in Lemma 2.2 satisfies

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

**Proof.** First, observe that

\[
\frac{\partial \ln(\lambda_1 + \frac{1}{3})}{\partial \mu_1} = \frac{\partial}{\partial \mu_1} \left[ \ln \int_{S^2} x^2 \exp(\mu_1 x^2 + \mu_2 y^2 + \mu_3 z^2) \, dS - \ln Z(\mu_1, \mu_2, \mu_3) \right]
\]

\[
= \int_{S^2} x^2 \exp(\mu_1 x^2 + \mu_2 y^2 + \mu_3 z^2) \, dS \left( \lambda_1 + 1 \right) \left( \frac{1}{3} \right)
\]

\[
= \left( \lambda_1 + \frac{1}{3} \right)^{-1} \left[ \int_{S^2} x^2 \rho_Q \, dS \int_{S^2} \rho_Q \, dS - \left( \int_{S^2} x^2 \rho_Q \, dS \right)^2 \right] > 0
\]

due to Schwarz’s inequality, and the fact that \( \rho_Q \) is not a perfect alignment of molecules as \( Q \) approaches the physical boundary. Hence as \( \lambda_1 \to -1/3 \), \( \mu_1 \) is strictly decreasing. It remains to prove \( \mu_1 \) 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 Lemma 2.2 and Lemma 2.4 we see that \( -M \leq \mu_1 \leq \mu_2 \leq \mu_3 \leq 2M \). As a consequence, together with the basic inequality

\[
\frac{2\theta}{\pi} \leq \sin \theta < \theta, \quad \forall 0 < \theta \leq \frac{\pi}{2}
\]

we obtain

\[
\lambda_1 + \frac{1}{3} = \int_{S^2} x^2 \rho_Q \, dS = \frac{\int_{S^2} x^2 \exp \{ (2\mu_1 + \mu_2)x^2 + (\mu_1 + 2\mu_2)y^2 \} \, dS}{\int_{S^2} \exp \{ (2\mu_1 + \mu_2)x^2 + (\mu_1 + 2\mu_2)y^2 \} \, dS}
\]
As a consequence, we conclude that which is a contradiction. Therefore, such lower bound $-M$ cannot exist, and the proof is complete. \hfill \square

Now we are ready to prove Theorem [1.3]

[Proof of Theorem 1.3]

\textbf{Proof. Case 1: $\lambda_1 = \lambda_2$.} In this case as $Q$ approaches is physical boundary we have

\[ Q = \begin{pmatrix}
-\frac{1}{3} + \varepsilon & 0 & 0 \\
0 & -\frac{1}{3} + \varepsilon & 0 \\
0 & 0 & 2/3 - 2\varepsilon
\end{pmatrix}, \quad \varepsilon \ll 1. \quad (2.7)
\]

By Lemmas 2.1 and 2.2 we get the optimal density functional $\rho_Q$ in (2.2) can be reformulated by

\[ \rho_Q = \frac{1}{Z} \exp \{ -3\nu(x^2 + y^2) \}, \quad \nu = -\mu_1, \quad Z = \int_{\Omega_2} \exp \{ -3\nu(x^2 + y^2) \} \, dS. \quad (2.8) \]

Henceforth the entropy reads

\[ \int_{\Omega_2} \rho_Q \ln \rho_Q \, dS = -\ln Z - 6\nu \varepsilon, \quad \text{with} \quad \varepsilon = \lambda_1 + \frac{1}{3}. \quad (2.9) \]

Using spherical coordinates, Dawson function as well as its asymptotic expansion for large $\eta$ as in [21],

\[ D_+(\eta) = e^{-\eta^2} \int_0^\eta e^t \, dt = \sum_{k=0}^{\infty} \frac{(2k-1)!!}{2^{k+1}(\eta^{2k+1})}, \quad \text{where} \quad (-1)!! = 1, \quad (2.10) \]

one can further derive

\[ Z = 4\pi \int_0^{\pi} \sin \theta \exp \{ -\xi \sin \theta \} \, d\theta \bigg|_{\xi = 3\nu} = 4\pi \int_0^1 \exp(-\xi + \xi t^2) \, dt \\
= \frac{4\pi}{\sqrt{\xi}} e^{-\xi} \int_0^{\sqrt{\xi}} e^{s^2} \, ds = \frac{4\pi}{\sqrt{\xi}} \sum_{k=0}^{\infty} \frac{(2k-1)!!}{2^{k+1}(\sqrt{\xi})^{2k+1}} = 2\pi \left[ 1 + \frac{1}{\xi} + O\left(\xi^{-3}\right) \right]. \]

Meanwhile, using spherical coordinates and (2.10) again we get

\[ \int_{\Omega_2} (x^2 + y^2) \exp \{ -\nu(x^2 + y^2) \} \, dS \\
= 4\pi \int_0^{\pi} \sin^3 \theta \exp \{ -\xi \sin \theta \} \, d\theta \bigg|_{\xi = 3\nu} = 4\pi \int_0^1 (1 - t^2) \exp(-\xi + \xi t^2) \, dt \\
= 4\pi \frac{d}{d\xi} \left( -e^{-\xi} \int_0^\xi e^{t^2} \, dt \right) = 4\pi \frac{d}{d\xi} \left( -e^{-\xi} \int_0^\xi e^{t^2} \, dt \right) = -4\pi \sum_{k=0}^{\infty} \frac{(2k-1)!!}{2^{k+1}(\sqrt{\xi})^{2k+2}} \\
= 2\pi \left[ 1 + O\left(\xi^{-3}\right) \right]. \]

As a consequence, we conclude that

\[ 2\left(\lambda_1 + \frac{1}{3}\right) = 2\varepsilon = \frac{\int_{\Omega_2} (x^2 + y^2) \exp \{ -\xi(x^2 + y^2) \} \, dS}{Z} = \frac{1}{\xi} + \frac{1}{\xi^2} + O\left(\xi^{-4}\right) \]

(2.11)
which plugged into (2.9) yields
\[
 f(Q) = \int_{S^2} \rho_\Omega \ln \rho_\Omega \, dS = - \ln Z - 6\varepsilon = - \ln 2\pi - \ln 2 - 1 - \ln \left( \lambda_1(Q) + \frac{1}{3} \right) + O(\xi^{-1}).
\] (2.12)
for sufficiently large \( \xi > 0 \).

**Case 2:** \( \lambda_1 < \lambda_2 \). To this end, we consider \( Q \) of the form
\[
 Q = \left( -\frac{1}{3} + \frac{\varepsilon^2}{3}, 0, 0, \lambda_2, 0, 0, \lambda_3 \right), \quad -\frac{1}{3} + \frac{\varepsilon^2}{3} < \lambda_2 \leq \lambda_3, \quad \lambda_2 + \lambda_3 = \frac{1}{3} - \frac{\varepsilon^2}{3}
\] (2.13)

Using the coordinate system
\[
\begin{cases}
  x = \cos \theta \\
  y = \sin \theta \sin \phi \\
  z = \sin \theta \cos \phi
\end{cases}
\]
we consider the domain
\[
 S^* = \{(1, \phi, \theta) \in S^2 \mid \phi \in [0, b) \cup [\pi - b, \pi] \cup [\pi, \pi + b] \cup [2\pi - b, 2\pi], \theta \in [\arccos \varepsilon, \pi - \arccos \varepsilon]\},
\] (2.14)
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
\[
\int_{S^2} \rho_\varepsilon \, dS = \frac{4}{8b\varepsilon} \int_0^b d\phi \int_{\arccos \varepsilon}^{\pi - \arccos \varepsilon} \sin \theta \, d\theta = 1,
\]
and the second moments with respect to \( \rho_\varepsilon \) are given by
\[
\begin{align*}
 &\int_{S^2} x^2 \rho_\varepsilon \, dS = \frac{1}{b\varepsilon} \int_0^b \int_{\arccos \varepsilon}^{\pi - \arccos \varepsilon} (\cos^2 \theta \sin^2 \theta) \, d\theta \, d\phi = \frac{\varepsilon^2}{3}, \\
 &\int_{S^2} y^2 \rho_\varepsilon \, dS = \frac{1}{b\varepsilon} \int_0^b \int_{\arccos \varepsilon}^{\pi - \arccos \varepsilon} (\sin^3 \theta \, d\theta) = \frac{\sqrt{b}}{4} - \sin \frac{2b}{4} \left( \varepsilon - \frac{\varepsilon^3}{3} \right) = \left( \frac{1}{2} - \frac{\sin 2b}{4b} \right) \left( 1 - \frac{\varepsilon^2}{3} \right), \\
 &\int_{S^2} z^2 \rho_\varepsilon \, dS = \frac{1}{b\varepsilon} \int_0^b \int_{\arccos \varepsilon}^{\pi - \arccos \varepsilon} \sin^3 \theta \, d\theta = \frac{\sqrt{b}}{4} + \sin \frac{2b}{4} \left( \varepsilon - \frac{\varepsilon^3}{3} \right) = \left( \frac{1}{2} + \frac{\sin 2b}{4b} \right) \left( 1 - \frac{\varepsilon^2}{3} \right), \\
 &\int_{S^2} xy \rho_\varepsilon \, dS = \int_{S^2} \frac{1}{2} \rho_\varepsilon \, dS = \int_{S^2} xz \rho_\varepsilon \, dS = 0.
\end{align*}
\]

Therefore, \( \rho_\varepsilon \in \mathcal{A}_R \) with
\[
 R = \left( \begin{array}{cccc}
 -\frac{1}{3} + \frac{\varepsilon^2}{3} & 0 & 0 & 0 \\
 0 & \frac{1}{6} - \frac{\sin 2b}{4b} - \frac{\sqrt{b}}{2} - \frac{\sin 2b}{4b} \frac{\varepsilon^2}{3} & 0 & 0 \\
 0 & 0 & \frac{1}{6} + \frac{\sin 2b}{4b} + \frac{\sqrt{b}}{2} + \frac{\sin 2b}{4b} \frac{\varepsilon^2}{3} & 0 \\
 \end{array} \right)
\]

We need to find a suitable \( 0 < b \leq \pi/2 \), such that
\[
 \frac{1}{6} - \frac{\sin 2b}{4b} - \left( \frac{1}{2} - \frac{\sin 2b}{4b} \right) \frac{\varepsilon^2}{3} = \lambda_2,
\]
which is equivalent to
\[
 \frac{\sin 2b}{2b} = 1 - \frac{2(\lambda_2 + \frac{1}{3})}{1 - \frac{\varepsilon^2}{3}}.
\] (2.15)
Note that $\sin(x)/x$ is monotone decreasing in $(0, \pi]$, with
\[
\lim_{x \to 0^+} \frac{\sin x}{x} = 1,
\]
hence we know (2.15) is solvable with $b \in (0, \pi/2]$. As a consequence, $R = Q$ and using mean value theorem we get
\[
x - \frac{x^3}{6} < \sin x, \quad \forall 0 < x \leq \pi; \quad \frac{1}{1 - y} > 1 + y, \quad \forall 0 < y < 1.
\]
Hence after inserting $x = 2b$, $y = \varepsilon^2/3$ into (2.15) we obtain
\[
1 - \frac{2b^2}{3} < \sin \frac{2b}{2b} < 1 - 2\left(1 + \frac{\varepsilon^2}{3}\right)\left(\lambda_2 + \frac{1}{3}\right),
\]
which further implies
\[
b^2 > (3 + \varepsilon^2)\left(\lambda_2 + \frac{1}{3}\right) > 3\left(\lambda_2 + \frac{1}{3}\right).
\]
In conclusion, we see $\rho_{\varepsilon} \in A_Q$ for $Q$ defined in (2.13), where $\lambda_1(Q) + 1/3 = \varepsilon^2/3$, and
\[
f(Q) \leq \int_{S^2} \rho_{\varepsilon} \log \rho_{\varepsilon} \, dS \leq \frac{8}{8b\varepsilon} \int_0^b \rho \int_{\theta_{\varepsilon}} \ln \frac{1}{8b\varepsilon} \sin \theta \, d\theta = -\ln(1 + \varepsilon) = -\ln 2 - \ln b - \ln \varepsilon
\]
\[
\leq -\ln 24 - \frac{1}{2} \ln \left(\lambda_1(Q) + \frac{1}{3}\right) + \frac{1}{2} \ln \left(\lambda_2(Q) + \frac{1}{3}\right).
\]
In all, the proof is complete after combining (2.12) and (2.18).

\textbf{Remark 2.1.} It is immediate to see from (1.10) and (1.11) that when $Q$ is “away from” the uniaxial structure (2.7), then $f(Q)$ is of the order $-1/2\ln(\lambda_1(Q) + 1/3)$.

\textbf{ Remark 2.2.} We guess that the associated lower bound for $f$ could be
\[
C_4 - \frac{1}{2} \ln \left(\lambda_1(Q) + \frac{1}{3}\right) - \frac{1}{2} \ln \left(\lambda_2(Q) + \frac{1}{3}\right) \leq f(Q),
\]
as $\lambda_1(Q) \to -1/3$ for some generic constant $C_4$. It is noted that (2.19) together with (1.9) will be of significance for numerics. Because the above inequality 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 $\lambda_1, \lambda_2$. Hence, by interpolating this well defined function, we can obtain an accurate numerical approximation of $f(Q)$.

3 Blowup rate of $\nabla f$

In this section we shall finish proof of Theorem 1.2, which plays an important role in the proof of regularity of solutions to the gradient flow generated by the Landau-de Gennes free energy with this singular potential $f$.

To this end, we shall study both the “radial” and “tangential” components of $\nabla f$ near the physical boundary of $Q$, and then focused on the estimate of its “radial” component. The main tool used in the estimate is basics of modified Bessel functions of first kind.

\textbf{Lemma 3.1.} For any physical $Q$-tensor of the form (2.1), suppose the associated Boltzmann distribution function of $f(Q)$ is given by (2.2). Then as $\lambda_1(Q) \to -1/3$, it holds
\[
\nabla_{rad} f(Q) = \sqrt{\frac{T}{2}} \partial_\varepsilon f(Q_\varepsilon) \varepsilon_{\xi=0} = -\sqrt{\frac{T}{2}} \mu_1, \tag{3.1}
\]
\[
\nabla_{tan} f(Q) = \sqrt{\frac{1}{2}} \partial_\varepsilon f(Q_\varepsilon) \varepsilon_{\xi=0} = -\sqrt{\frac{T}{2}} (\mu_1 + 2\mu_2). \tag{3.2}
\]
Here $\nabla_{rad} f(Q)$ (resp. $\nabla_{tan} f(Q)$) is defined in (3.3) (resp. in (3.4)) below.
Proof. Recall from \([\text{[1]}\) Lemma C.1 that for a given physical \(Q\)-tensor of the form \(\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\), its projection on the physical boundary is

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

and their distance is

\[
d(Q) \equiv \|Q - Q^\perp\|_F = \frac{\sqrt{6}}{2}(\lambda_1 + \frac{1}{3}).
\]

Let us denote

\[
Q^\perp_\varepsilon \equiv \begin{pmatrix} \lambda_1 - \varepsilon & 0 & 0 \\ 0 & \lambda_2 + \frac{\varepsilon}{2} & 0 \\ 0 & 0 & \lambda_3 + \frac{\varepsilon}{2} \end{pmatrix}, \quad Q^\parallel_\varepsilon \equiv \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 + \varepsilon & 0 \\ 0 & 0 & \lambda_3 - \varepsilon \end{pmatrix},
\]

and refer to \(Q^\perp_\varepsilon - Q\) (resp. \(Q^\parallel_\varepsilon - Q\)) as the radial (resp. tangential direction), and note that these two directions are orthogonal in the sense that their inner product

\[
(Q^\perp_\varepsilon - Q) : (Q^\parallel_\varepsilon - Q) = \begin{pmatrix} -\varepsilon & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & -\varepsilon \end{pmatrix} : \begin{pmatrix} 0 & 0 & 0 \\ 0 & -\varepsilon & 0 \\ 0 & 0 & 0 \end{pmatrix} = 0.
\]

**Step 1: radial component.** We first calculate

\[
\nabla_{\text{rad}} f(Q) \equiv \lim_{\varepsilon \to 0} \frac{f(Q^\perp_\varepsilon) - f(Q)}{\|Q^\perp_\varepsilon - Q\|_F} = \sqrt{\frac{2}{3}} \frac{\partial f(Q^\perp_\varepsilon)}{\partial \varepsilon} \bigg|_{\varepsilon = 0}.
\]

Let us denote \(\rho^\perp_\varepsilon\) the associated Boltzmann distribution function of \(f(Q^\perp_\varepsilon)\)

\[
\rho^\perp_\varepsilon = \exp \left\{ \mu^\perp_1(\varepsilon)x^2 + \mu^\perp_2(\varepsilon)y^2 + \mu^\perp_3(\varepsilon)z^2 \right\}, \quad (x, y, z) \in S^2, \quad \mu^\perp_1(\varepsilon) + \mu^\perp_2(\varepsilon) + \mu^\perp_3(\varepsilon) = 0,
\]

\[
Z^\perp_\varepsilon = \int_{S^2} \exp \left\{ \mu^\perp_1(\varepsilon)x^2 + \mu^\perp_2(\varepsilon)y^2 + \mu^\perp_3(\varepsilon)z^2 \right\} dS.
\]

Clearly, \(\rho_0\) (resp. \(\mu_i, i = 1, 2, 3\)) is the optimal Boltzmann distributions (resp. Lagrange multipliers) associated to \(Q\). Let

\[
\lambda^\perp_1(\varepsilon) = \lambda_1 - \varepsilon, \quad \lambda^\perp_2(\varepsilon) = \lambda_2 + \frac{\varepsilon}{2}, \quad \lambda^\perp_3(\varepsilon) = \lambda_3 + \frac{\varepsilon}{2},
\]

then direct computations give

\[
\frac{\partial f(Q^\perp_\varepsilon)}{\partial \varepsilon} = -\frac{\partial \ln Z^\perp_\varepsilon}{\partial \varepsilon} + \frac{3}{\varepsilon} \sum_{i=1}^{\mu^\perp_i(\varepsilon)} \left[ \lambda^\perp_i(\varepsilon) + \frac{1}{3} \right]
\]

\[
= -\frac{\partial \ln Z^\perp_\varepsilon}{\partial \mu_i^\perp(\varepsilon)} \mu_i^\perp(\varepsilon) \left( \lambda^\perp_i(\varepsilon) + \frac{1}{3} \right) + \sum_{i=1}^{\mu_i^\perp(\varepsilon)} \left[ \lambda^\perp_i(\varepsilon) + \frac{1}{3} \right] + \sum_{i=1}^{\mu_i^\perp(\varepsilon)} \mu_i^\perp(\varepsilon) \lambda^\perp_i(\varepsilon) = -\mu_i^\perp(\varepsilon) + \frac{\mu_2^\perp(\varepsilon) + \mu_3^\perp(\varepsilon)}{2}
\]

which gives \((3.3)\) after evaluating at \(\varepsilon = 0\).

**Step 2: tangential component.** We proceed to calculate

\[
\nabla_{\text{tan}} f(Q) \equiv \lim_{\varepsilon \to 0} \frac{f(Q^\parallel_\varepsilon) - f(Q)}{\|Q^\parallel_\varepsilon - Q\|_F} = \sqrt{\frac{2}{3}} \frac{\partial f(Q^\parallel_\varepsilon)}{\partial \varepsilon} \bigg|_{\varepsilon = 0}.
\]

Analogously, we denote \(\rho^\parallel_\varepsilon\) the associated Boltzmann distribution function of \(f(Q^\parallel_\varepsilon)\)

\[
\rho^\parallel_\varepsilon = \exp \left\{ \mu^\parallel_1(\varepsilon)x^2 + \mu^\parallel_2(\varepsilon)y^2 + \mu^\parallel_3(\varepsilon)z^2 \right\}, \quad (x, y, z) \in S^2, \quad \mu^\parallel_1(\varepsilon) + \mu^\parallel_2(\varepsilon) + \mu^\parallel_3(\varepsilon) = 0,
\]
Proposition 3.1. where \( \nabla \) the upper bound and lower bound of

\[
\text{Proof of Theorem 1.2} \quad \text{The proof of Theorem 1.2 lies in the following two propositions, which provides}
\]

\[
\text{Proof.} \quad \text{To begin with, we see from Lemma 3.1 that}
\]

\[
\frac{\partial f(Q)}{\partial \varepsilon} = \frac{\partial \ln Z}{\partial \mu} \varepsilon + \sum_{i=1}^{3} \mu_i \left( \frac{\lambda_i \varepsilon + 1}{3} \right) + \sum_{i=1}^{3} \mu_i \lambda_i \varepsilon = \mu_2 \varepsilon - \mu_3 \varepsilon,
\]

which leads to (3.2) after evaluating at \( \varepsilon = 0 \).

As an immediate consequence, we have

**Corollary 3.1.** As \( \lambda_1(Q) \to -1/3 \), it holds

\[
1 \leq \frac{\| \nabla f(Q) \|_F}{\| \nabla_{rad} f(Q) \|} \leq 2.
\]

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

\[
\| \nabla f(Q) \|_F^2 = \| \nabla_{rad} f(Q) \|^2 + \| \nabla_{tan} f(Q) \|^2 = \frac{3}{2} \mu_1^2 + \frac{1}{2} (\mu_1 + 2 \mu_2)^2.
\]

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

\[
3 \mu_1 \leq \mu_1 + 2 \mu_2 \leq 0,
\]

which implies

\[
\| \nabla f(Q) \|_F^2 \leq \frac{3}{2} \mu_1^2 + \frac{1}{2} (3 \mu_1)^2 = 6 \mu_1^2,
\]

and further together with (3.1) yields

\[
1 \leq \frac{\| \nabla f(Q) \|_F^2}{\| \nabla_{rad} f(Q) \|^2} \leq \frac{6 \mu_1^2}{2 \mu_1^2} = 4.
\]

**Remark 3.1.** It follows from Lemma 3.1 and Corollary 3.1 that, to estimate the blowup rate of \( \| \nabla f(Q) \|_F \) as \( \lambda_Q \to -1/3 \), it suffices to estimate \( \mu_1 \).

[Proof of Theorem 1.2] The proof of Theorem 1.2 lies in the following two propositions, which provides the upper bound and lower bound of \( \nabla f(Q) \), respectively.

**Proposition 3.1.** For any physical \( Q \)-tensor of the form (2.1), as \( \lambda_1(Q) \to -1/3 \), there exists a suitably small constant \( \varepsilon_0 > 0 \), such that

\[
\| \nabla f(Q) \| \geq \frac{C_1}{\lambda_1 + \frac{1}{3}}, \quad \text{provided} \quad 0 < \lambda_1 + \frac{1}{3} < \varepsilon_0,
\]

where \( C_1 \) is given in (1.13).

**Proof.** To begin with, we see from Lemma 3.1 that

\[
\| \nabla f(Q) \| \geq \| \nabla_{rad} f(Q) \|^2 = \frac{3}{2} \mu_1^2,
\]

where \( \mu_1 \) is the Lagrange multiplier associated with the Boltzmann distribution function of \( f(Q) \) given in (2.2). Hence it remains to estimate \( \mu_1 \) in terms of \( \lambda_1(Q) + 1/3 \), as \( \lambda_1(Q) \to -1/3 \). From (2.2) we know that

\[
\lambda_1(Q) + \frac{1}{3} = \frac{\int_{S^2} x^2 \exp \left\{ (2 \mu_1 + \mu_2) x^2 + (\mu_1 + 2 \mu_2) y^2 \right\} dS}{\int_{S^2} \exp \left\{ (2 \mu_1 + \mu_2) x^2 + (\mu_1 + 2 \mu_2) y^2 \right\} dS}
\]
\[
\int_{S^{2}} x^2 \exp(-Ax^2 - By^2) \, dS = \frac{\int_{S^{2}} x^2 \exp(-Ax^2 - By^2) \, dS}{\int_{S^{2}} \exp(-Ax^2 - By^2) \, dS}.
\tag{3.8}
\]

Here in (3.8) we denote \( A = -(2\mu_1 + \mu_2), B = -(\mu_1 + 2\mu_2), \) by (2.2). Lemmas 2.1 and 2.2, it is immediate to see
\[
A \gg 1, \quad B \geq 0.
\tag{3.9}
\]

**Step 1: Estimating the numerator in (3.8)**

Using the coordinate system
\[
v(x, \theta) = (x, \sqrt{1 - x^2} \cos \theta, \sqrt{1 - x^2} \sin \theta), \quad 0 \leq x \leq 1, 0 \leq \theta \leq 2\pi,
\tag{3.10}
\]
whose surface element is given by \( \left| \frac{\partial v}{\partial x} \times \frac{\partial v}{\partial \theta} \right| = 1, \) we get
\[
\int_{S^{2}} x^2 \exp(-Ax^2 - By^2) \, dS = 2 \int_{S^{2} \cap \{x \geq 0\}} x^2 \exp(-Ax^2 - By^2) \, dS
\]
\[
= 2 \int_{0}^{\pi} \int_{0}^{1} y^2 e^{-Ax^2} \left[ \int_{0}^{2\pi} e^{-B(1-x^2) \cos^2 \theta} \, d\theta \right] \, dx.
\tag{3.11}
\]

Note that the zeroth modified Bessel function of first kind \( I_0 \) is represented by
\[
I_0(\xi) = \frac{1}{\pi} \int_{0}^{\pi} \exp(\xi \cos \theta) \, d\theta = \sum_{n=0}^{\infty} \frac{1}{(m!)^2} \left( \frac{\xi}{2} \right)^{2m},
\tag{3.12}
\]
and \( I_0(\xi) = I_0(-\xi), \) hence we have
\[
\int_{0}^{2\pi} e^{-B(1-x^2) \cos^2 \theta} \, d\theta = \exp \left\{ \frac{-B(1-x^2)}{2} \right\} \int_{0}^{2\pi} \exp \left\{ \frac{-B(1-x^2) \cos(2\theta)}{2} \right\} \, d\theta
\]
\[
\quad \overset{(\eta = 2\theta)}{=} \exp \left\{ \frac{-B(1-x^2)}{2} \right\} \int_{0}^{2\pi} \exp \left\{ \frac{-B(1-x^2) \cos(\eta)}{2} \right\} \, d\eta
\]
\[
= \exp \left\{ \frac{-B(1-x^2)}{2} \right\} \left[ \int_{0}^{\pi} \exp \left\{ \frac{-B(1-x^2) \cos(\eta)}{2} \right\} \, d\eta + \int_{0}^{\pi} \exp \left\{ \frac{-B(1-x^2) \cos(\eta)}{2} \right\} \, d\eta \right]
\]
\[
= I_0 \left( \frac{-B(1-x^2)}{2} \right) + I_0 \left( \frac{B(1-x^2)}{2} \right) = 2I_0 \left( \frac{B(1-x^2)}{2} \right).
\]

Inserting the above identity into (3.11), together with (3.9), we obtain
\[
\int_{S^{2}} x^2 \exp(-Ax^2 - By^2) \, dS = 2 \int_{0}^{1} x^2 e^{-Ax^2} \exp \left\{ \frac{-B(1-x^2)}{2} \right\} I_0 \left( \frac{B(1-x^2)}{2} \right) \, dx
\]
\[
\geq 4\pi e^{-1} \int_{0}^{1} x^2 e^{-Ax^2} \exp \left\{ \frac{-B(1-x^2)}{2} \right\} I_0 \left( \frac{B(1-x^2)}{2} \right) \, dx
\tag{3.13}
\]

Meanwhile, since \( I_0 \)
\[
\frac{d}{d\xi} [e^{-\xi} I_0(\xi)] = e^{-\xi} [I_1(\xi) - I_0(\xi)] = e^{-\xi} \int_{0}^{\pi} [\cos \theta - 1] \exp(\xi \cos \theta) \, d\theta < 0,
\]
the function \( \xi \mapsto e^{-\xi} I_0(\xi) \) is strictly decreasing. Correspondingly we have
\[
x \mapsto \exp \left\{ \frac{-B(1-x^2)}{2} \right\} I_0 \left( \frac{B(1-x^2)}{2} \right)
\]
is strictly increasing for \( x \in [0, 1].\)
\[
\tag{3.14}
\]
By virtue of (3.14), we get
\[
\inf_{x \in [a, 1/\sqrt{A}]} \exp \left\{ \frac{-B(1-x^2)}{2} \right\} I_0 \left( \frac{B(1-x^2)}{2} \right) = \exp \left\{ \frac{-B}{2} \right\} I_0 \left( \frac{B}{2} \right),
\]

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which together with (3.13) implies
\[
\int_{S^2} x^2 \exp(-Ax^2 - By^2) dS \geq \frac{4\pi}{e} \exp \left\{ -\frac{B}{2} \right\} I_0 \left( \frac{B}{2} \right) \int_0^1 x^2 dx = \frac{4\pi}{3e} \exp \left\{ -\frac{B}{2} \right\} I_0 \left( \frac{B}{2} \right) A^{-\frac{1}{2}}. \tag{3.15}
\]

**Step 2: Estimating the denominator in (3.8)**

Similar to the last step, we have
\[
\int_{S^2} \exp(-Ax^2 - By^2) dS = 4\pi \int_0^1 e^{-Ax^2} \exp \left\{ -\frac{B(1-x^2)}{2} \right\} I_0 \left( \frac{B(1-x^2)}{2} \right) dx
\]
\[
= 4\pi \int_0^1 e^{-Ax^2} \exp \left\{ -\frac{B(1-x^2)}{2} \right\} I_0 \left( \frac{B(1-x^2)}{2} \right) dx
\]
\[
+ 4\pi \int_0^1 e^{-Ax^2} \exp \left\{ -\frac{B(1-x^2)}{2} \right\} I_0 \left( \frac{B(1-x^2)}{2} \right) dx. \tag{3.16}
\]

Recall (3.14), then we see
\[
\int_0^1 e^{-Ax^2} \exp \left\{ -\frac{B(1-x^2)}{2} \right\} I_0 \left( \frac{B(1-x^2)}{2} \right) dx \leq \int_0^1 e^{-\frac{A}{4} x^2} dx \leq \frac{2-\sqrt{2}}{2} e^{-\frac{A}{4}},
\]
\[
\int_0^\infty e^{-Ax^2} \exp \left\{ -\frac{B(1-x^2)}{2} \right\} dx \leq \exp \left\{ -\frac{B}{4} \right\} I_0 \left( \frac{B}{4} \right) \int_0^\infty e^{-Ax^2} dx
\]
\[
\leq \exp \left\{ -\frac{B}{4} \right\} I_0 \left( \frac{B}{4} \right) \int_0^\infty e^{-Ax^2} dx = \exp \left\{ -\frac{B}{4} \right\} I_0 \left( \frac{B}{4} \right) \sqrt{\frac{\pi}{4A}}.
\]

Since \(\xi \to e^{-\xi/4} I_0(\xi/4)\) is decreasing, while \(\xi \to I_0(\xi/4)\) is increasing for \(\xi \geq 0\), and \(B \leq A\), \(A \gg 1\), there exists a computable, universal constant \(A_0\) such that
\[
\frac{2-\sqrt{2}}{2} e^{-\frac{A}{4}} \leq \exp \left\{ -\frac{A}{4} \right\} \sqrt{\frac{\pi}{4A}} \leq \exp \left\{ -\frac{A}{4} \right\} I_0 \left( \frac{A}{4} \right) \sqrt{\frac{\pi}{4A}} \leq \exp \left\{ -\frac{B}{4} \right\} I_0 \left( \frac{B}{4} \right) \sqrt{\frac{\pi}{4A}}, \quad \forall A \geq A_0.
\]

To sum up, we conclude
\[
\int_{S^2} \exp(-Ax^2 - By^2) dS \leq 4\pi \exp \left\{ -\frac{B}{4} \right\} I_0 \left( \frac{B}{4} \right) \sqrt{\frac{\pi}{A}}, \quad \forall A \geq A_0 \tag{3.17}
\]

**Step 3: Combining both estimates in (3.8)**

We get immediately from (3.15) and (3.17) that
\[
\lambda_1(Q) + \frac{1}{3} = \frac{1}{3e^{3\sqrt{\pi A}}} \exp \left\{ -\frac{B}{4} \right\} I_0 \left( \frac{B}{4} \right), \quad \forall A \geq A_0 \tag{3.18}
\]

Since \(-3\mu_1 \geq A \geq -\frac{3}{2} \mu_1\), it remains to bound the last fraction in (3.18). Since \(e^{-\xi} I_0(\xi) > 0, \forall \xi \geq 0\), and equal to 1 at \(\xi = 0\), it suffices to show
\[
\liminf_{\xi \to +\infty} \exp \left\{ -\frac{B}{4} \right\} I_0 \left( \frac{B}{4} \right) > 0 \tag{3.19}
\]

The Taylor expansion of \(e^{-\xi} I_0(\xi)\), for \(\xi > 1\), is (21)
\[
e^{-\xi} I_0(\xi) = \frac{1}{\sqrt{2\pi}} \left[ \xi^{-\frac{3}{2}} + \frac{1}{8} \xi^{-\frac{5}{2}} + \frac{9}{128} \xi^{-\frac{7}{2}} + O(\xi^{-\frac{9}{2}}) \right],
\]

hence the limit in (3.19) is equal to \(1/\sqrt{2}\). Thus one can establish from (3.18) and the fact \(-3\mu_1 \geq A \geq -\frac{3}{2} \mu_1\) that
\[
\lambda_1(Q) + \frac{1}{3} \geq \frac{1}{A} \frac{1}{3e^{3\sqrt{\pi A}}} \inf_{\xi \geq 0} e^{-\xi} I_0 \left( \frac{B}{2} \right), \quad \forall A \geq A_0,
\]

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which further gives

$$\lambda_1(Q) + \frac{1}{3} \geq -\frac{1}{\mu_1} \frac{1}{9e^\sqrt{\pi} \xi \geq 0} e^{-\xi} I_0(\xi),$$

provided \( \mu_1 < -\frac{2A_0}{3} \). (3.20)

In view of Lemma 2.2, there exists a suitably small constant \( \varepsilon_0 > 0 \), such that

$$\mu_1 < -\frac{2A_0}{3},$$

provided \( 0 < \lambda_1(Q) + \frac{1}{3} < \varepsilon_0 \).

In all, using (1.12) we conclude that from (3.20) that

$$\|\nabla f(Q)\|_F \geq |\nabla_{rad} f(Q)| \geq \frac{\sqrt{6}}{2} \mu_1 \geq \frac{C_1}{\lambda_1(Q) + \frac{1}{3}},$$

provided \( 0 < \lambda_1(Q) + \frac{1}{3} < \varepsilon_0 \), completing the proof.

**Proposition 3.2.** For any physical \( Q \)-tensor of the form (2.1), as \( \lambda_1(Q) \to -1/3 \), there exists a suitably small constant \( \varepsilon_0 > 0 \), such that

$$\|\nabla f(Q)\|_F \leq \frac{C_2}{\lambda_1 + \frac{1}{3}},$$

provided \( 0 < \lambda_1 + \frac{1}{3} < \varepsilon_0 \), (3.22)

where \( C_2 \) is given in (1.12).

**Proof.** In contrast to the proof of Proposition 3.1, we need to obtain suitable upper bound on the numerator of (3.8), but lower bound on the denominator of (3.8).

**Step 1: Estimating the numerator in (3.8)**

Using the coordinate system (3.10), similar to the proof of Proposition 3.1 one can establish

$$\int_{\mathbb{R}^3} x^2 \exp(-Ax^2 - By^2) \, dS = 4\pi \int_0^1 x^2 e^{-Ax^2} \exp \left\{ -\frac{B(1 - x^2)}{2} \right\} I_0 \left[ \frac{B(1 - x^2)}{2} \right] \, dx$$

$$= 4\pi \int_0^\frac{1}{4} x^2 e^{-Ax^2} \exp \left\{ -\frac{B(1 - x^2)}{2} \right\} I_0 \left[ \frac{B(1 - x^2)}{2} \right] \, dx$$

$$+ 4\pi \int_{\frac{1}{4}}^1 x^2 e^{-Ax^2} \exp \left\{ -\frac{B(1 - x^2)}{2} \right\} I_0 \left[ \frac{B(1 - x^2)}{2} \right] \, dx,$$

$$\leq 4\pi (J_1 + J_2).$$

In view of (3.14), we get

$$J_2 \leq \int_{\frac{1}{4}}^1 x^2 e^{-Ax^2} \, dx = \frac{2 - \sqrt{2}}{2} e^{-\frac{A}{4}},$$

(3.24)

and

$$J_1 \leq \int_0^{\frac{1}{4}} x^2 e^{-Ax^2} \exp \left\{ -\frac{B}{4} \right\} I_0 \left( \frac{B}{4} \right) \, dx = \exp \left\{ -\frac{B}{4} \right\} I_0 \left( \frac{B}{4} \right) \left[ -\frac{e^{-\frac{A}{2} + 1}}{2A} \right]$$

$$\leq \exp \left\{ -\frac{B}{4} \right\} I_0 \left( \frac{B}{4} \right) \left[ -\frac{e^{-\frac{A}{2} + 1}}{2A} \right]$$

$$= \exp \left\{ -\frac{B}{4} \right\} I_0 \left( \frac{B}{4} \right) \left[ -\frac{e^{-\frac{A}{2} + 1}}{2A} \right].$$

(3.25)

Since \( B \leq A, \) and \( \xi \mapsto e^{-\xi} I_0(\xi) \) is decreasing, we have

$$0 < \frac{e^{-\xi}}{\exp \left\{ -\frac{A}{4} \right\} I_0 \left( \frac{A}{4} \right) \sqrt{\pi} \frac{A}{4} \sqrt{\pi}} \leq \frac{e^{-\xi}}{\exp \left\{ -\frac{A}{4} \right\} I_0 \left( \frac{A}{4} \right) \sqrt{\pi} \frac{A}{4} \sqrt{\pi}} = \frac{4A^{-\frac{1}{2}}}{e^{\frac{A}{2}} I_0 \left( \frac{A}{4} \right) \sqrt{\pi}} \to 0, \text{ as } A \to +\infty.$$
Hence there exists a computable constant $A_0 > 0$, such that

$$J_1 + J_2 \leq \frac{2 - \sqrt{7}}{2} e^{-\frac{3}{2}} + \exp \left( - \frac{B}{4} \right) I_0 \left( \frac{B}{4} \right) \frac{\sqrt{e}}{2 \sqrt{2A}} \leq \exp \left( - \frac{B}{4} \right) I_0 \left( \frac{B}{4} \right) \frac{\sqrt{e}}{A} \sqrt{2}, \quad \forall A > A_0,$$

which inserts into (3.23) yields

$$\int_{S^2} x^2 \exp(-Ax^2 - By^2) dS \leq 4\pi (J_1 + J_2) \leq 4\pi \exp \left( - \frac{B}{4} \right) I_0 \left( \frac{B}{4} \right) \frac{\sqrt{e}}{A} \sqrt{2}, \quad \forall A > A_0.$$  \hspace{1cm} (3.26)

**Step 2: Estimating the denominator in (3.23)**

Using (3.20), the coordinate system (3.10) and (3.14), we get

$$\int_{S^2} \exp(-Ax^2 - By^2) dS = 4\pi \int_{0}^{1} e^{-Ax^2} \exp \left( - \frac{B(1 - x^2)}{2} \right) I_0 \left( \frac{B(1 - x^2)}{2} \right) dx$$

$$\geq 4\pi \int_{0}^{1} e^{-Ax^2} \exp \left( - \frac{B(1 - x^2)}{2} \right) I_0 \left( \frac{B(1 - x^2)}{2} \right) dx$$

$$\geq \frac{4\pi}{e\sqrt{A}} \exp \left( - \frac{B}{2} \right) I_0 \left( \frac{B}{2} \right).$$  \hspace{1cm} (3.27)

**Step 3: Completing the proof**

Combining (3.20) and (3.27), we see that

$$\lambda_1(Q) + \frac{1}{3} \leq \frac{\exp \left( - \frac{B}{4} \right) I_0 \left( \frac{B}{4} \right)}{e\sqrt{A}} \frac{\sqrt{2}}{A} \leq \exp \left( - \frac{B}{4} \right) I_0 \left( \frac{B}{4} \right) A \sup_{\xi \geq 0} \frac{\exp \left( - \frac{\xi}{4} \right) I_0 \left( \frac{\xi}{4} \right)}{\exp \left( - \frac{\xi}{4} \right) I_0 \left( \frac{\xi}{4} \right)}, \quad \forall A > A_0 \hspace{1cm} (3.28)$$

where

$$\sup_{\xi \geq 0} \frac{\exp \left( - \frac{\xi}{4} \right) I_0 \left( \frac{\xi}{4} \right)}{\exp \left( - \frac{\xi}{4} \right) I_0 \left( \frac{\xi}{4} \right)} \geq \frac{I_0(0)}{I_0(0)} = 1.$$

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

$$-\mu_1 \leq -2\mu_1 - \mu_2 = A \leq \frac{1}{\lambda_1(Q) + \frac{1}{3}} \exp \left( - \frac{B}{4} \right) I_0 \left( \frac{B}{4} \right) \exp \left( - \frac{\xi}{4} \right) I_0 \left( \frac{\xi}{4} \right), \quad \forall A > A_0.$$

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

$$\|\nabla f(Q)\|_F \leq 2|\nabla rad f(Q)| \leq -\sqrt{6} \mu_1 = \frac{C_2}{\lambda_1(Q) + \frac{1}{3}},$$

where $C_2$ is given in Theorem 1.12, completing the proof. \hfill \Box

**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.

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