\(\Gamma\)-convergence of a mean-field model of a chiral doped nematic liquid crystal to the Oseen–Frank description of cholesterics

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Abstract

Systems of elongated molecules, doped with small amounts of molecules lacking mirror symmetry can form macroscopically twisted cholesteric liquid crystal phases. The aim of this work is to rigorously derive the Oseen–Frank model of cholesterics from a more fundamental model concerned with pairwise molecular interactions. A non-local mean-field model of the two-species nematic host/chiral dopant mixture is proposed, and it is shown that Oseen–Frank’s elastic free energy for cholesteric liquid crystals can be obtained in a simultaneously large-domain and dilute-dopant asymptotic regime. By techniques of \(\Gamma\)-convergence, it is shown that in the asymptotic limit, dopant–dopant interactions are negligible, the Frank constants and nematic host order parameter are unperturbed by the presence of dopant, but the mirror asymmetry of the dopant–host interaction leads to a macroscopically twisted ground state. The constant of proportionality between the helical wavenumber and dopant concentration, the helical twisting power (HTP), can be explicitly found through such an analysis, with a nonlinear temperature dependence. Depending on the relative strengths of the host–host and host–dopant interactions, it is shown that HTP may increase or decrease with temperature.

Keywords: Oseen–Frank, cholesteric liquid crystals, helical twisting power, \(\Gamma\)-convergence

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1. Introduction

1.1. Motivation

It has long been known that systems of asymmetric molecules can form mesophases outside of the classical solid–liquid–gas trichotomy [7]. The earliest classification of such phases described the nematic, smectic and cholesteric phases [12]. In the nematic phase molecules admit (local) orientational ordering but no positional ordering. In the smectic phase molecules admit orientational and periodic one-dimensional positional ordering, but are translationally disordered within two orthogonal dimensions. Thirdly there is the cholesteric phase, which resembles a nematic on small length scales but forms helical structures over larger length scales. The macroscopic chirality of these helical structures is associated with a corresponding microscopic chirality of the constituent molecules. Early attempts to study cholesteric liquid crystals considered purer systems of chiral molecules, though in more recent years however it has become commonplace to consider multi-species mixtures, where an achiral host system that would naturally form a nematic phase is doped by a small quantity (often as little as 1%–2%) of a chiral dopant. These are typically far more stable and have attracted a wealth of interest. From a practical perspective, cholesterics and complex materials with cholesteric character have found applications due to their tunable optical properties, allowing them to be exploited for many purposes such as displays [18], e-paper [35], mechanically-tunable lasing [10], and smart windows [3]. The purpose of this work is to provide a rigorous derivation of the Oseen–Frank model for cholesterics consisting of achiral nematic host with chiral dopant by considering it as a simultaneous large-domain and dilute dopant limit of a more fundamental model based on long-range, attractive, molecular interactions. Furthermore, we relate the corresponding interaction potentials to material constants appearing in the macroscopic models. We advise the reader to the notation section in appendix A.1.

1.2. Continuum theories of nematics

Nematic liquid crystals are systems of rod like molecules where the centre of mass of particles is disordered, but their long axis, often described by a unit vector \( p \in S^2 \) respecting the head-to-tail symmetry \( p \sim -p \), admits local ordering. The Landau–de Gennes model of nematics describes a domain \( \Omega \subset \mathbb{R}^3 \) of nematic liquid crystal by its Q-tensor, a traceless symmetric matrix that is the normalised second order moment of the local orientation distribution function \( \int_{S^2} (p \otimes p - \frac{1}{3} I) f(x,p) \, dp \). We define the set \( \text{Sym}_0(3) \) to be the traceless symmetric matrices, explicitly,

\[
\text{Sym}_0(3) = \{ Q \in \mathbb{R}^{3 \times 3} : \text{Tr}(Q) = 0, \, Q = Q^T \}.
\]

(2)

Taking \( Q \) to be our order parameter and representative of local orientational ordering, we consider a free energy minimisation, with the free energy generally of the form

\[
\int_{\Omega} W(\nabla Q(x), Q(x)) + \psi_B(Q(x)) \, dx,
\]

(3)

where \( W, \psi_B \) are frame-indifferent functions, \( \psi_B \) is the ‘bulk’ contribution to the energy, and \( W \) the ‘elastic’ contribution, satisfying \( W(0,Q) = 0 \) for all \( Q \). For simplicity, \( W \) is typically...
taken to be quadratic in $\nabla Q$, where the requirement of frame invariance leads to the commonly used energy

$$W(\nabla Q, Q) = \frac{L_1}{2} Q_{ij,j} Q_{kk} + \frac{L_2}{2} Q_{ij,j} Q_{lj,k} + \frac{L_3}{2} Q_{ij,j} Q_{lj,k} + \frac{L_4}{4} Q_{ik} Q_{lj,k} Q_{ik,j},$$  \hspace{1cm} (4)

where Einstein notation is employed, and indices after commas denote derivatives in the corresponding coordinate direction. Such models may be justified by a phenomenological Landau expansion, or inferred from molecular models as gradient expansions [14]. To the author’s knowledge, however, the passage from mean-field models to Landau–de Gennes has yet to be understood by means of a rigorous proof, instead typically employing truncated series expansions.

Much contemporary work has been devoted to understanding the behaviour of the Landau–de Gennes Q-tensor model in the large domain limit, particularly in the ‘one-constant’ case where $L_1 = L_3 = L_4 = 0$ [13, 24, 27]. In such a regime, the bulk energy becomes highly penalised, requiring that in the limit $Q(x) \in \arg \min \psi_B$ pointwise, which is a set of matrices of the form $s_0 (n \otimes n - \frac{1}{4} I)$, where $s_0 > 0$ is a constant depending on various material parameters, and any $n \in S^2$. As $n$ is the only degree of freedom, in the case when $Q = s_0 (n \otimes n - \frac{1}{4} I)$ for some $n \in W^{1,2}(\Omega, S^2)$, the energy reduces to the Oseen–Frank energy [11],

$$\int_\Omega \frac{K_{11}}{2} (\nabla \cdot n)^2 + \frac{K_{22}}{2} (n \cdot \nabla \times n)^2 + \frac{K_{33}}{2} |n \times \nabla \times n|^2 \, dx. \hspace{1cm} (5)$$

It should be noted that while $Q$ respects $n$, $-n$ equivalence, a unit vector field does not, and this has the consequence that such an $n$ does not always exist in $W^{1,2}(\Omega, S^2)$ [2, 4]. The constants $K_{11}, K_{22}, K_{33}$, relating to the penalisation of splay, twist and bend deformations, respectively, are known as the Frank constants. The Frank constants are related to the constants $L_i$ in the Landau–de Gennes free energy. There is also a so-called ‘saddle-splay’ term depending only on Dirichlet boundary conditions which we will neglect for this work. The Oseen–Frank model too can be justified phenomenologically by arguing that the energy must be frame invariant, respect $n$, $-n$ symmetry, be minimised at $\nabla n = 0$, and be well approximated by a quadratic in $\nabla n$ in the small deformation regime.

While much work has been done on the rigorous asymptotics of obtaining Oseen–Frank from Landau–de Gennes, there has been recent interest in obtaining Oseen–Frank directly from molecular models as a large domain limit. This has included asymptotic descriptions of solutions to the Euler–Lagrange equation and minimisers [20], convergence of gradient flow-type energies [21] and $\Gamma$-convergence [32]. We will continue in this approach with this work, but for the case of cholesteric liquid crystals formed of a two-species system.

1.3. Cholesteric liquid crystals

Cholesteric liquid crystals differ from nematics in that their ground states are twisted helical structures. The Oseen–Frank description of cholesterics amounts to the introduction of a term linear in $\nabla n$, so that the energy becomes

$$\frac{1}{2} \int_\Omega K_{11} (\nabla \cdot n(x))^2 + K_{22} (n(x) \cdot \nabla \times n(x) + q)^2 + K_{33} |n(x) \times \nabla \times n(x)|^2 \, dx,$$

where $q$ is a pseudo-scalar describing the wavenumber of the ground state. As $q$ is both a pseudo-scalar (that is, a scalar which changes sign under spatial inversion) and a material
constant, this implies that the system must have some kind of intrinsic chirality, which results from molecular chirality. The extra term linear in $\nabla n$ has a corresponding analogue in the Landau–de Gennes model given by

$$\frac{L_5}{2} \epsilon_{ikl} Q_{0l} Q_{0k}.$$  

(7)

The ground state of (6) in the absence of frustrating boundary conditions is given by configurations of the form

$$n(x) = \cos(qx \cdot e_3)e_1 + \sin(qx \cdot e_3)e_2$$

(8)

in a right-handed orthonormal basis $e_1, e_2, e_3$, so $e_1 \times e_2 = e_3$. While $n$ is $\frac{2\pi}{q}$ periodic in the $e_3$ direction, as $n$ and $-n$ represent the same configuration, the periodicity of this structure is $\frac{\pi}{q}$. In the case of an achiral host with chiral dopant, we expect $q$ to be roughly proportional to the concentration of dopant in dilute systems. The constant of proportionality is called the helical twisting power (HTP). The HTP is generally readily measurable experimentally, however difficult to predict. HTP may vary heavily between the same host across different dopants and vice versa, and HTP may be either increasing or decreasing as a function of temperature (see e.g. [18]). There have been numerous attempts to estimate helical pitch from molecular properties from a theoretical standpoint in both single-species [5, 15, 33] and doped systems [8, 16, 29].

In this work we obtain an explicit expression for the HTP depending on various material constants, host concentration, and scalar order parameters of the host and dopant. These scalar order parameters can themselves be explicitly derived from temperature, host number density and material constants. The novelty of our approach against previous work is twofold. Firstly, the problem is qualitatively a singular perturbation problem, phrased in the language of $\Gamma$-convergence. Secondly, we use few ansatzes on our solutions, with features such as the uniaxiality of solutions and the dopant being (locally) aligned with the host being proven from the analysis. These twofold components are of course related, as the commonly taken ansatzes are those expected to hold in large domains. The fact that they are proven to hold exactly in our analysis is a consequence of the asymptotic regime considered. The homogenised nature of our limiting model also provides simpler conclusions.

### 1.4. Outline of the paper and main results

Section 2 is devoted to the derivation of a mean-field model for chiral doped nematics in a periodic domain. In the usual mean-field spirit, we describe the energy as a competition between pairwise interactions and entropy, in a two-species mixture of host and dopant. Initially, the model is described in terms of orientation distribution functions of each species, however by taking an ansatz that the pairwise interaction energy is bilinear in the effective molecular orientation descriptor tensors, through symmetry arguments and an exact moment closure procedure the model is reduced to a simpler, macroscopic energy defined in terms of the $Q$-tensors of the host and dopant species. Significantly, host–dopant and dopant–dopant interactions display chirality through antisymmetric terms in the interaction energy. We then consider an asymptotic scaling corresponding to a large domain with dilute dopant. This leads to the energy $F_\epsilon$ as defined in definition 2.9. The energy admits a small parameter $\epsilon > 0$ which is both proportional to the concentration of dopant and inversely proportional to the sample size. This particular scaling is relevant as it is expected that the periodicity of the cholesteric ground state should be $\frac{\pi}{h\rho_D}$ where $h$ is the HTP and $\rho_D$ is the number density of dopant. Thus
if we expect to see structures of the same length scale as the domain, we require $\frac{1}{\rho_D}$ to be comparable to the sample size.

Before proceeding with a rigorous $\Gamma$-convergence argument, we first provide a heuristic argument in section 3, motivating the more precise analysis in later sections. By formally replacing non-local finite differences with gradients, we obtain a Landau–de Gennes flavoured free energy in (54) for the host and dopant Q-tensors. By neglecting high order terms and minimising the free energy at successive orders of the expansion parameter $\epsilon$, we formally obtain the Oseen–Frank free energy for cholesterics, though symmetry arguments are required to reduce the expression into the classical form, and describe the Frank constants in terms of integrals of molecular interactions and the equilibrium scalar order parameters. As the expansion argument is purely heuristic, in section 4 we provide a precise argument in the language of $\Gamma$-convergence for periodic boundary conditions. It is shown that the limiting free energy formally obtained can be described as the $L^2$-$\Gamma$ limit of $\mathcal{F}_\epsilon$ as $\epsilon \to 0$, which gives us the main theorem of this work, theorem 4.19.

Compactness and lower semicontinuity results from [32] are of use in the proof strategy. The key ingredients are to prove that the dopant–dopant interaction terms provide an asymptotically vanishing contribution to the energy, which is a consequence of the dilute regime we consider. The main qualitative difference from the arguments in [32] are due to the presence of two energy scales within the bulk-type energy, requiring more care to be taken in providing estimates and recovery sequences, and understanding the interactions between the two macroscopic order parameters.

While the $\Gamma$-convergence argument provides the limiting energy, the representation of the energy is not in the classical form. In section 5 we employ symmetry arguments to reduce to a more classical representation. The Frank constants for one-component systems were given in terms of molecular interactions in [32], which are unaffected in this analysis. It thus remains to obtain an expression for the HTP that results from this analysis. Our analysis provides the following equation, that the HTP satisfies

$$h = -\frac{\tilde{\beta}}{\rho_H K_{22}} \frac{s_c}{s_0}.$$  \hspace{1cm} (9)

Here $\tilde{K}_{22}$ and $\tilde{\beta}$ are material constants, and can be thought of as the temperature and concentration independent components of the splay Frank constant and the coefficient of $n \cdot \nabla \times n$, given explicitly in terms of integrals of host–host and host–dopant interactions, respectively. The scalars $s_0$ and $s_c$ are the scalar order parameters of the host and dopant, respectively, and $\rho_H$ is the number density of the host. While they are nonlinearly dependent on many model parameters, explicit expressions for $s_c, s_0$ are available, and the temperature dependence of the HTP is encoded within their ratio. A dimensionless contribution to the HTP, $\tilde{h} = \frac{h}{s_0}$, is the only part that is explicitly temperature dependent. It is determined entirely by two dimensionless parameters $\alpha$, representing the relative strength of host–host and host–dopant bulk interactions, and a rescaled temperature $\tau$. This relationship is numerically tractable, and a plot of $\tilde{h}$ against $\alpha, \tau$ is presented in figure 2. Significantly, for $\alpha > 1$, that is when host–host interactions are stronger than host–dopant, we see HTP increasing as a function of temperature. When $\alpha < 1$, HTP becomes a decreasing function of temperature. At the critical value $\alpha = 1$, when host–host and host–dopant interactions are comparable, it is proven that HTP is independent of temperature. It should be noted that due to differences in formulation, it is difficult to compare the given expressions to existing literature such as [8, 16, 29]. The closest formulation is that of [29], which lacks (explicit) thermal dependence nor a bulk energy, and
admits several qualitatively different modelling assumptions. However beyond these inconsistencies, there appears to be a qualitative consistency, for example their expression would admit a similar \( \frac{1}{T} \) temperature dependence arising from relevant integrations of interaction energies, should their assumptions be sufficiently tweaked to match those of this work.

2. The model

Let \( \Omega \) denote a subset of \( \mathbb{R}^3 \) containing nematic host \( (H) \) and a chiral dopant \( (D) \). We presume both species to be elongated molecules, and statistically well described by their long axis alone. We describe the system through two functions, \( f_H, f_D : \Omega \to \mathcal{P}(S^2) \). For \( x \in \Omega \), \( f_X(x, \cdot) \) is interpreted as the probability distribution describing the distribution of long axis orientations of species \( X = H, D \) near \( x \). The molecules need not necessarily admit perfect cylindrical symmetry, but are assumed to statistically be well described by such a distribution on their long axis. This difference will be essential in the description of the chiral contributions to the energy, and will be expanded upon in remark 2.3. We assume that the number density of long axis. This difference will be essential in the description of the chiral contributions to the energy, and will be expanded upon in remark 2.3. We assume that the number density of nematic \( \rho_H > 0 \) and dopant \( \rho_D > 0 \) to be constant in space. Denote by \( -\tilde{K}_{XY}(z,p,q) \) the interaction energy between two particles of species \( X, Y \) with orientations \( p, q \) (respectively), and centres of mass separated by a vector \( z \in \mathbb{R}^3 \). We then presume the free energy, up to additive constants irrelevant to our analysis, to be of the form

\[
k_B T \int_{\Omega \times S^2} \rho_H f_H(x,p) \ln f_H(x,p) + \rho_D f_D(x,p) \ln f_D(x,p) \, d(x,p)
- \int_{\Omega \times S^2} \int_{\Omega \times S^2} \frac{\rho_H}{2} \tilde{K}_{HH}(x-y,p,q) f_H(x,p) f_H(y,q) \, d(x,p) \, d(y,q)
- \int_{\Omega \times S^2} \int_{\Omega \times S^2} \rho_H \rho_D \tilde{K}_{HD}(x-y,p,q) f_H(x,p) f_D(y,q) \, d(x,p) \, d(y,q)
- \int_{\Omega \times S^2} \int_{\Omega \times S^2} \frac{\rho_D}{2} \tilde{K}_{DD}(x-y,p,q) f_D(x,p) f_D(y,q) \, d(x,p) \, d(y,q).
\]

Each line corresponds, respectively, to entropy, host–host interactions, host–dopant interactions, and dopant–dopant interactions. The factors of \( \frac{1}{2} \) in the second and fourth line are to avoid double-counting of interactions, \( k_B \) denotes the Boltzmann constant and \( T > 0 \) temperature.

This model is a Maier–Saupe-type model [23] for a two species system, permitting spatial variations at constant number density of both species. We will be considering the case of long-range, attractive interactions, a fact expressed mathematically by a positivity requirement on the interactions \( \tilde{K}_{XY} \). The model is aesthetically similar to that of Onsager [28], although the latter is model based on short-range, repulsive interactions, which as a purely steric model admits no temperature dependence.

2.1. Pairwise interactions

Here and throughout the sequel, \( \cdot \) will denote the inner product of tensors of equal rank, so that for vectors \( u \cdot v = u_i v_i \), for 2-tensors \( A \cdot B = A_{ij} B_{ij} = \text{Tr}(AB^T) \), and for 4-tensors \( X \cdot Y = X_{ijkl} Y_{ijkl} \). The norms used for vectors and 2-tensors correspond to these inner products, the Euclidean norm for vectors \( |u| = \sqrt{u \cdot u} \) and Frobenius norm for 2-tensors \( |A| = \sqrt{A \cdot A} \).

For each choice of \( X, Y \), \( \tilde{K}_{XY} \) must be frame indifferent, so that for all rotations \( R \in \text{SO}(3) \)

\[
\tilde{K}_{XY}(Rz, Rp, Rq) = \tilde{K}_{XY}(z, p, q).
\]
Furthermore, the head-to-tail symmetry requirement gives
\[ \tilde{K}_{XY}(z,p,q) = \tilde{K}_{XY}(z,\pm p,\pm q). \] (12)
Inversion symmetry (or lack thereof) can be characterised by the difference
\[ \tilde{K}'_{XY}(z,p,q) = \frac{1}{2} \tilde{K}_{XY}(z,p,q) - \frac{1}{2} \tilde{K}_{XY}(-z,-p,-q) = \frac{1}{2} \tilde{K}_{XY}(z,p,q) - \frac{1}{2} \tilde{K}_{XY}(-z,p,q). \] (13)
\( \tilde{K}'_{XY} \neq 0 \) implies a lack of inversion symmetry, and thus at least one of the molecules must be chiral. We also consider the symmetric part of the interaction,
\[ \tilde{K}_{XY}^\sigma(z,p,q) = \frac{1}{2} \tilde{K}_{XY}(z,p,q) + \frac{1}{2} \tilde{K}_{XY}(-z,p,q). \] (14)
so that \( \tilde{K}_{XY} = \tilde{K}_{XY}^\sigma + \tilde{K}'_{XY} \). If \( X, Y \) are both representative of achiral molecules, we expect \( \tilde{K}_{XY} = \tilde{K}_{XY}^\sigma \).

We define the microscopic order parameter for \( p \in S^2 \) as the traceless symmetric matrix
\[ \sigma(p) = p \otimes p - \frac{1}{4} I. \] For simplicity we presume that \( \tilde{K}_{XY}(z,p,q) \) is bilinear in \( \sigma(p), \sigma(q) \). That is, we assume that for every \( z \in \mathbb{R}^3 \), we have a linear operator \( \tilde{K}_{XY}(z) : \text{Sym}_0(3) \to \text{Sym}_0(3) \) so that
\[ \tilde{K}_{XY}(z,p,q) = \tilde{K}_{XY}(z)\sigma(p) \cdot \sigma(q). \] (15)
This is evocative to the London dispersion forces [22], which describes the leading order contribution to long-range interactions as a function bilinear in the molecular polarisibility tensors. In our case of (statistically) axially symmetric molecules, the molecular polarisibility tensors will be of the form \( \alpha_{iso} I + \alpha_{ani} \sigma(p) \), where \( \alpha_{iso}, \alpha_{ani} \) are constants representing the average polarisibility and anisotropy of polarisibility, respectively.

This may be viewed as a truncated spherical harmonic expansion in \( p \cdot q \) of an arbitrary interaction energy. Similar techniques may be applicable to other finite-order spherical harmonics expansions, with appropriate technical assumptions, though for simplicity we restrict ourselves to the form of (15) in this work, since Q-tensors are familiar objects with easily understood geometry via their eigenvalue decomposition. Furthermore, such an interaction energy provides many explicit results that would not be as clear for general interaction energies, such as the possible symmetric invariants (propositions 2.1 and 2.2), and significantly we have explicit information on the ground state manifold \( \mathcal{M} \) (to be defined in definition 4.7). This information is essential for providing quantitative information on the \( \Gamma^\ast \)-limit of the energy, and would likely have to be replaced with more broad, qualitative information if the interaction energy were more complex.

Due to frame indifference, we find that the condition (11) is in fact quite restrictive on the form of \( \tilde{K}_{XY}(z) = \frac{1}{4} \{ \tilde{K}_{XY}(z) + \tilde{K}_{XY}(-z) \} \).

**Proposition 2.1.** Let \( \tilde{K}_{XY}^\sigma(z) : \text{Sym}_0(3) \to \text{Sym}_0(3) \) satisfy the conditions in (11)–(15). Then there exist functions \( z \mapsto k_i(z), i = 1, 2, 3, \) depending only on \( |z| \), so that
\[ \tilde{K}_{XY}^\sigma(z)A = k_1(z)A + k_2(z)(Az \otimes z + z \otimes Az) + k_3(z)(Az \cdot z)z \otimes z - \frac{A z \cdot z}{3} (2k_2(z) + k_3(z)|z|^2) I. \] (16)

**Proof.** Deferred to appendix A.2.

As the host is achiral, we assume \( \tilde{K}_\text{host}(z,p,q) = 0 \). However the host–dopant and dopant–dopant interactions must contain some chiral contribution, as the dopant is chiral.
For simplicity, we take \( \tilde{K}_{XY}(z,p,q) \) to depend linearly on the microscopic order parameters \( \sigma(p), \sigma(q) \) also, so that
\[
\tilde{K}_{HD}(z,p,q) = \tilde{K}_{H}(z)\sigma(p) \cdot \sigma(q),
\]
\[
\tilde{K}_{DD}(z,p,q) = \tilde{K}_{D}(z)\sigma(p) \cdot \sigma(q),
\]
for some tensors \( \tilde{K}_{H}(z), \tilde{K}_{D}(z) \), which must have odd symmetry. Much like the achiral contributions to the interaction energy, this gives us a restrictive condition on the type of operator permitted.

**Proposition 2.2.** Let \( \tilde{K}_{X}(z) : \text{Sym}_0(3) \rightarrow \text{Sym}_0(3) \) satisfy the conditions in (11)–(15). Then there exist scalar functions \( f_1, f_2 : \mathbb{R}^3 \rightarrow \mathbb{R} \), so that \( f_i(z) \) depends only on \( |z| \), so that
\[
\tilde{K}_{X}(z)A = f_1(z)(AW - WA) - f_2(z)(WAW^2 - W^2AW),
\]
where \( W \) is the skew-symmetric tensor defined by \( Wx = z \times x \) for all \( x \in \mathbb{R}^3 \). Equivalently, \( W_{ij} = -\epsilon_{ijk}z_k \) with \( \epsilon_{ijk} \) the Levi-Civita tensor.

**Proof.** Deferred to appendix A.3 \( \square \)

We note this includes the form considered in [33] as a particular case.

**Remark 2.3.** We note that for molecules to be chiral, they necessarily cannot have cylindrical symmetry, raising questions of the validity of such an expression for a chiral interaction described only by the uniaxial microscopic order parameters \( \sigma(p) \). This is however justified in [33] for one-component systems and exploited in [29] for two-component systems, by considering low-symmetry chiral molecules with a well-defined long axis. It is assumed that all orientations with the long axis pointing in the same direction are equally probable. We could describe this by saying that if the long-axis of the molecule in a reference frame is \( e_1 \), and \( \rho \in \mathcal{P}(\text{SO}(3)) \) is the (local) distribution of orientations of the molecule with respect to this reference frame, then \( \rho(R) = \rho(Re_1) \) for some \( \rho \in \mathcal{P}(\mathbb{S}^2) \). Averaging electrostatic interactions between systems of such molecules can obtain components in an interaction energy such as (18), where chiral contributions to the energy remain, despite being described by an order parameter \( \sigma(p) \) that cannot encode chirality.

### 2.2. Entropy and order parameters

In this subsection, including proposition 2.4, we freely quote results from [1, 26, 31].

Let \( \mathcal{P}(\mathbb{S}^2) = \{ f \in L^1(\mathbb{S}^2) : f \geq 0 \ \text{a.e.}, \int_{\mathbb{S}^2} f(p) \, dp = 1 \} \). Let \( f \in \mathcal{P}(\mathbb{S}^2) \). We define the Q-tensor of \( f \) to be
\[
Q = \int_{\mathbb{S}^2} f(p)\sigma(p) \, dp = \int_{\mathbb{S}^2} f(p) \left( p \otimes p - \frac{1}{3}I \right) \, dp.
\]
\( Q \) is thus a traceless, symmetric, \( 3 \times 3 \) matrix. Furthermore, the constraint that \( f \) be an \( L^1 \) probability distribution forces the constraint that the smallest eigenvalue of \( Q \), \( \lambda_{\text{min}}(Q) \), be strictly greater than \( -\frac{1}{3} \). The tracelessness conditions means a given Q-tensor can be one of three flavours:
• $Q = 0$, in which case we say $Q$ is isotropic, and representative of a disordered system.
• $Q$ has exactly two distinct eigenvalues, in which case we say $Q$ is uniaxial, and representative of a system of molecules roughly aligned with axial symmetry. We can decompose $Q = s (n \otimes n - \frac{1}{3} I)$ for a scalar order parameter $s \neq 0$, and Oseen–Frank’s director $n \in S^2$. If $s > 0$, molecules are roughly aligned along $\pm n$, while if $s < 0$, molecules typically lie in the plane orthogonal to $n$.
• $Q$ has three distinct eigenvalues, in which case $Q$ is biaxial, and representative of an ordered system with lower symmetry than a uniaxial system.

Typically we expect to find nematic liquid crystals in a uniaxial state, with positive scalar order parameter [9, 26, 34]. The order parameter $s$ can be taken as representative of the degree of ordering of the system, with $s = 1$ corresponding to a perfectly ordered state.

The eigenvalue constraint that $\lambda_{\min}(Q) > -\frac{1}{3}$ means that not all traceless symmetric matrices are physically meaningful. In fact, given a traceless symmetric matrix $Q$, there exists some $L^1$ distribution $f$ with finite Shannon entropy so that (19) holds if and only if $\lambda_{\min}(Q) > -\frac{1}{3}$.

Thus we define the set of physical $Q$-tensors to be

$$Q = \left\{ Q \in \mathbb{R}^{3 \times 3} : Q = Q^T, \text{Tr}(Q) = 0, \lambda_{\min}(Q) > -\frac{1}{3} \right\}. \quad (20)$$

This is an open bounded convex set, and its closure $\bar{Q}$ simply consists of traceless symmetric matrices with $\lambda_{\min}(Q) \geq -\frac{1}{3}$. We can define a macroscopic analogue of entropy, $\psi_s : Q \to \mathbb{R}$ by

$$\psi_s(Q) = \min_{f \in A_Q} \int_{S^2} f(p) \ln f(p) \, dp, \quad (21)$$

where the admissible set $A_Q$ is defined as

$$A_Q = \left\{ f \in \mathcal{P}(S^2) : \int_{S^2} f(p) \sigma(p) \, dp = Q \right\}. \quad (22)$$

Heuristically, $\psi_s$ is a macroscopic analogue of the entropic contribution to the energy, obtained by a maximum entropy assumption. It satisfies the following properties.

**Proposition 2.4.** Let $\psi_s : Q \to \mathbb{R}$ be defined as in (21). Then the following hold.

1. $\psi_s$ is strongly convex, $C^\infty$, frame indifferent, and blows up to $+\infty$ as $\lambda_{\min}(Q) \to -\frac{1}{3}$.
2. The derivative of $\psi_s$, denoted $\Lambda : Q \to \text{Sym}_0(3)$, is a frame indifferent bijection.
3. For every $Q \in Q$ there exists a unique minimiser $f^Q$ of the minimisation problem in (21) given by

$$f^Q(p) = \frac{1}{Z_Q} \exp(\Lambda(Q) p \cdot p), \quad (23)$$

where $Z_Q > 0$ is a normalisation constant.
4. $\Lambda^{-1} : \text{Sym}_0(3) \to Q$ satisfies

$$\Lambda^{-1}(A) = \left( \int_{S^2} \exp(A p \cdot p) \, dp \right)^{-1} \int_{S^2} \sigma(p) \exp(A p \cdot p) \, dp. \quad (24)$$

5. $\psi_s$ can be written in terms of $\Lambda$ as $\psi_s(Q) = \Lambda(Q) \cdot Q - \ln \int_{S^2} \exp(\Lambda(Q) p \cdot p) \, dp$. 


6. Let $k \in \mathbb{R}$, and define $\psi_{b}\psi_{b}(Q) = \psi_{b}(Q) - \frac{1}{2} |Q|^{2}$. Then there exists some $k^*$ so that if $k < k^*$, $\psi_{b}$ is minimised only at $Q = 0$, while for $k > k^*$, $\psi_{b}$ is minimised at all $Q$-tensors of the form $s(k) \{ n \otimes n - \frac{1}{4} I \}$ for any $n \in \mathbb{S}^{2}$, and some $s : (k^*, \infty) \to \mathbb{R}$.

7. Let $k > k^*$, $e_1, e_2, e_3$ be an orthonormal basis of $\mathbb{R}^{3}$, and $Q = s(k)\sigma(e_1)$. Then there exists a constant $c_k > 0$ so that if $\xi = s\sigma(e_1) + t(e_2 \otimes e_2 - e_3 \otimes e_3)$, then $\nabla^{2}\psi_{b}(Q) \xi \cdot \xi \geq c_k(s^{2} + t^{2})$ for $s, t [19, \text{proposition } 4.2]$.

2.3. The total energy—macroscopic form

Recalling the energy (10), we now simplify it to a macroscopic form via an exact moment closure. The main technical issues in making the arguments precise are that the constraints $f_{k}(x, \cdot) \in \mathcal{P}([0,1])$ and the definition of the Q-tensor involve integrals of $L^{1}$ functions over a zero measure set, for which one must invoke Fubini’s theorem.

First, we define the macroscopic Q-tensors $Q, \xi : \Omega \to \mathbb{Q}$ corresponding to the orientations of Host and Dopant molecules (respectively), by

$$
Q(x) = \int_{\mathbb{S}^{2}} \sigma(p) f_{h}(x, p) \, dp,
$$

$$
\xi(x) = \int_{\mathbb{S}^{2}} \sigma(p) f_{d}(x, p) \, dp. \tag{25}
$$

We now reduce the interaction terms to integrals involving only the moments. The argument follows for all terms, so we provide the calculation for only the host–dopant interaction. Using these definitions, we may simplify the pairwise interaction terms as follows

$$
\int_{\Omega \times \mathbb{S}^{2}} \int_{\Omega \times \mathbb{S}^{2}} K_{HH}(x - y, p, q) f_{h}(x, p) f_{d}(y, q) \, dx \, dp \, dy \, dq
$$

$$
= \int_{\Omega \times \mathbb{S}^{2}} \int_{\Omega \times \mathbb{S}^{2}} (K_{HH}^{*}(x - y) + K_{Hh}(x - y)) \cdot (\sigma(p) \otimes \sigma(q)) f_{h}(x, p) f_{d}(y, q) \, dx \, dp \, dy \, dq
$$

$$
= \int_{\Omega \times \Omega} (K_{HH}^{*}(x - y) + K_{Hh}(x - y)) \cdot \left( \int_{\mathbb{S}^{2}} \sigma(p) f_{h}(x, p) \, dp \otimes \int_{\mathbb{S}^{2}} \sigma(q) f_{d}(y, q) \, dq \right) \, dx \, dy
$$

$$
= \int_{\Omega} \int_{\Omega} (K_{HH}^{*}(x - y) + K_{Hh}(x - y)) \cdot (Q(x) \otimes \xi(y)) \, dx \, dy
$$

$$
= \int_{\Omega} \int_{\Omega} (K_{HH}^{*}(x - y)Q(x) \cdot \xi(y) + K_{Hh}(x - y)Q(x) \cdot \xi(y)) \, dx \, dy. \tag{26}
$$

Analogous arguments give

$$
\int_{\Omega \times \mathbb{S}^{2}} \int_{\Omega \times \mathbb{S}^{2}} K_{DD}(x - y, p, q) f_{d}(x, p) f_{d}(y, q) \, dx \, dp \, dy \, dq
$$

$$
= \int_{\Omega} \int_{\Omega} K_{DD}^{*}(x - y)Q(x) \cdot Q(y) \, dx \, dy,
$$

$$
\int_{\Omega \times \mathbb{S}^{2}} \int_{\Omega \times \mathbb{S}^{2}} K_{hD}(x - y, p, q) f_{h}(x, p) f_{d}(y, q) \, dx \, dp \, dy \, dq
$$

$$
= \int_{\Omega} \int_{\Omega} K_{hD}^{*}(x - y)\xi(x) \cdot \xi(y) + K_{hD}(x - y)\xi(x) \cdot \xi(y) \, dx \, dy. \tag{27}
$$

As the interaction terms depend only on the macroscopic Q-tensors, we may aim to replace the energy with a simpler, equivalent analogue involving only macroscopic variables. To this end, we provide the following proposition.
Proposition 2.5. Let $F : \mathcal{L}^\infty(\Omega, \mathbb{R}^3) \rightarrow \mathbb{R} \cup \{\pm \infty\}$ be given by

$$F(\xi) = \int_\Omega k_B T\rho_0 \psi(\xi) + k_B T\rho_0 \psi_0(\xi) \, dx - \frac{\rho_0^2}{2} \int_\Omega \int_\Omega K_{BB}(x-y)\xi(x) \cdot \xi(y) + K_{\rho}(x-y)\xi(x) \cdot \xi(y) \, dy \, dx$$

$$- \rho_0^2 \int_\Omega \int_\Omega K_{BB}(x-y)Q(x) \cdot Q(y) \, dy \, dx - \rho_0 \mu H \int_\Omega \int_\Omega \left( K_{BB}(x-y)Q(x) \cdot Q(y) + K_{\rho}(x-y)Q(x) \cdot \xi(y) \right) \, dy \, dx.$$ \hspace{1cm} (28)

Let $G : L^1(\Omega, \mathcal{P}(\mathbb{S}^2)^2) \rightarrow \mathbb{R} \cup \{\pm \infty\}$ be given by

$$G(f_\mu, f_\rho) = \int_{\Omega \times \mathbb{S}^2} k_B T\rho_0 f_\mu(x, p) \ln f_\mu(x, p) + k_B T\rho_0 f_\rho(x, p) \ln f_\rho(x, p) \, d(x, p)$$

$$- \frac{\rho_0^2}{2} \int_\Omega \int_\Omega K_{BB}(x-y)\xi(x) \cdot \xi(y) + K_{\rho}(x-y)\xi(x) \cdot \xi(y) \, dy \, dx$$

$$- \frac{\rho_0^2}{2} \int_\Omega \int_\Omega K_{BB}(x-y)Q(x) \cdot Q(y) \, dy \, dx - \rho_0 \mu H \int_\Omega \int_\Omega \left( K_{BB}(x-y)Q(x) \cdot Q(y) + K_{\rho}(x-y)Q(x) \cdot \xi(y) \right) \, dy \, dx,$$ \hspace{1cm} (29)

with $Q(x) = \int_{\mathbb{S}^2} \sigma(p) f_\mu(x, p) \, dp$, $\xi(x) = \int_{\mathbb{S}^2} \sigma(p) f_\rho(x, p) \, dp$.

If $(f_\mu, f_\rho)$ is an $L^1$-local minimising pair for $G$, then $f_\mu = f_\rho^0, f_\rho = f_\rho^0$, and $(Q, \xi)$ is an $L^1$-local minimising pair for $F$. Furthermore, if $(Q, \xi)$ is an $L^1$-local minimising pair for $F$, then $(f_\rho^0, f_\rho^0)$ is an $L^1$-local minimising pair for $G$.

Proof. Proof deferred to appendix A.4. \hfill $\square$

This leads us to the equivalent macroscopic free energy to be considered in this work,

$$\int_\Omega k_B T\rho_0 \psi(\xi) + k_B T\rho_0 \psi_0(\xi) \, dx - \frac{\rho_0^2}{2} \int_\Omega \int_\Omega K_{BB}(x-y)\xi(x) \cdot \xi(y) + K_{\rho}(x-y)\xi(x) \cdot \xi(y) \, dy \, dx$$

$$- \rho_0^2 \int_\Omega \int_\Omega K_{BB}(x-y)Q(x) \cdot Q(y) \, dy \, dx - \rho_0 \mu H \int_\Omega \int_\Omega \left( K_{BB}(x-y)Q(x) \cdot Q(y) + K_{\rho}(x-y)Q(x) \cdot \xi(y) \right) \, dy \, dx.$$ \hspace{1cm} (30)

2.4. Scaling, periodic domains and non-dimensionalisation

Consider the energy (30) in the case when $\Omega = \mathbb{R}^3$, with a configuration $\frac{2\pi}{\tau}$-periodic in each of the coordinate dimensions. Let $\mathbb{T}^3$ denote the (flat) torus in 3D with unit sides $2\pi$. The energy per unit cell is then given by

$$\int_{\mathbb{T}^3} k_B T\rho_0 \psi(\xi) + k_B T\rho_0 \psi_0(\xi) \, dx - \frac{\rho_0^2}{2} \int_{\mathbb{T}^3} \int_{\mathbb{T}^3} K_{BB}(x-y)\xi(x) \cdot \xi(y) + K_{\rho}(x-y)\xi(x) \cdot \xi(y) \, dy \, dx$$

$$- \rho_0^2 \int_{\mathbb{T}^3} \int_{\mathbb{T}^3} K_{BB}(x-y)Q(x) \cdot Q(y) \, dy \, dx - \rho_0 \mu H \int_{\mathbb{T}^3} \int_{\mathbb{T}^3} \left( K_{BB}(x-y)Q(x) \cdot Q(y) + K_{\rho}(x-y)Q(x) \cdot \xi(y) \right) \, dy \, dx.$$ \hspace{1cm} (31)

Note in the double integrals, the inner integral is over all of $\mathbb{R}^3$ as molecules interact not only with molecules in their unit cell, but all cells due to the non-locality. We now perform a change of variables, $x = \frac{x'}{\tau}, y = \frac{y'}{\tau}, Q' (x') = Q(x), \xi' (x') = \xi(x)$. Then $Q', \xi'$ are $2\pi$-periodic in the coordinate directions. The energy can thus be written as
\[ \mathcal{F} = \frac{1}{\epsilon^3} \int_{\mathbb{R}^3} k_0 T \rho_0 \psi_\epsilon(Q'(x')) + k_0 T \rho_0 \psi_\epsilon(\xi'(x')) \, dx' \]

\[ - \frac{\rho_0}{2 \epsilon^2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} K^\epsilon_D \left( \frac{x' - y'}{\epsilon} \right) \xi'(x') \cdot \xi'(y') + K_D \left( \frac{x' - y'}{\epsilon} \right) \xi'(x') \cdot \xi'(y') \, dx' \, dy' \]

\[ - \frac{\rho_0}{2 \epsilon^2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} K^\epsilon_H \left( \frac{x' - y'}{\epsilon} \right) Q'(x') \cdot Q'(y') \, dx' \, dy' \]

\[ - \frac{\rho_0}{\epsilon^2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \left( K^\epsilon_D \left( \frac{x' - y'}{\epsilon} \right) \xi'(x') \cdot \xi'(y') + K_D \left( \frac{x' - y'}{\epsilon} \right) \xi'(x') \cdot \xi'(y') \right) \, dx' \, dy'. \]

We will consider an asymptotically dilute regime, so that \( \rho_0 = \rho_0 \rho D \) for some \( \rho_0 > 0 \), independent of \( \epsilon \). Then we consider the rescaled free energy \( \frac{\mathcal{F}}{\rho_0 k_0 T} \), which satisfies

\[ \frac{\mathcal{F}}{\rho_0 k_0 T} = \frac{1}{\epsilon^3} \int_{\mathbb{R}^3} \psi_\epsilon(Q'(x')) + \rho_0 \psi_\epsilon(\xi'(x')) \, dx' \]

\[ - \frac{\rho_0}{2 \epsilon^2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} K^\epsilon_D \left( \frac{x' - y'}{\epsilon} \right) \xi'(x') \cdot \xi'(y') + K_D \left( \frac{x' - y'}{\epsilon} \right) \xi'(x') \cdot \xi'(y') \, dx' \, dy' \]

\[ - \frac{\rho_0}{2 \epsilon^2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} K^\epsilon_H \left( \frac{x' - y'}{\epsilon} \right) Q'(x') \cdot Q'(y') \, dx' \, dy' \]

\[ - \frac{\rho_0}{\epsilon^2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \left( K^\epsilon_D \left( \frac{x' - y'}{\epsilon} \right) \xi'(x') \cdot \xi'(y') + K_D \left( \frac{x' - y'}{\epsilon} \right) \xi'(x') \cdot \xi'(y') \right) \, dx' \, dy'. \]

We now redefine our operators into a dimensionless analogue, as

\[ \frac{\rho_0}{k_0} k^\epsilon_D \rightarrow K_D, \quad \frac{\rho_0}{k_0} k^\epsilon_H \rightarrow K_H, \]

\[ \frac{\rho_0}{k_0} K^\epsilon_D \rightarrow K_D, \quad \frac{\rho_0}{k_0} K^\epsilon_H \rightarrow K_H. \]

This leads us to the energy which we will aim to minimise,

\[ \mathcal{F}(Q, \xi) = \int_{\mathbb{R}^3} \psi_\epsilon(Q) + \frac{1}{\epsilon^3} \rho_0 \psi_\epsilon(\xi) - c, \, dx \]

\[ - \frac{1}{2 \epsilon^2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} K^\epsilon_H \left( \frac{x' - y'}{\epsilon} \right) Q(x') \cdot Q(y') + 2 \rho_0 \epsilon K_D \left( \frac{x' - y'}{\epsilon} \right) Q(x') \cdot \xi(y') + \rho_0^2 \epsilon^2 K_D^\epsilon \left( \frac{x' - y'}{\epsilon} \right) \xi(x') \cdot \xi(y') \, dx' \, dy' \]

\[ - \frac{1}{\epsilon^2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \rho_0 \epsilon K_D \left( \frac{x' - y'}{\epsilon} \right) \xi(x') \cdot \xi(y') + \frac{1}{2} \rho_0^2 \epsilon^2 K_D^\epsilon \left( \frac{x' - y'}{\epsilon} \right) \xi(x') \cdot \xi(y') \, dx' \, dy'. \]

The constant \( c \) is to be determined later and does not affect the minima, and will be chosen so that the ‘bulk’ contribution to the energy has minimum zero.

We now include some technical assumptions on the interaction terms, which will be required for the precise analysis in section 4. Note constants \( C, C_1, C_2 \) will be used to represent generic positive constants and may change from line to line, here and throughout the paper. 

**Assumption 2.6.** The functions \( K_{XY}, K_X \) are \( L^1(\mathbb{R}^3) \), frame indifferent functions for all choices of \( X, Y \) as \( H, D \). Furthermore, they satisfy the following inequalities. There exists positive constants \( C_1, C_2 \), and a non-negative frame indifferent\(^2\) function \( g \in L^1(\mathbb{R}^3) \) with \( \int_{\mathbb{R}^3} |x|^2 g(x) \, dx < +\infty \) so that

\[ ^2 \text{By frame indifferent we mean that } g(z) \text{ depends only on } |z|. \]
\[ C_1 g(\epsilon) \left( |A|^2 + |B|^2 - 1 \right) \]
\[ <K_{II}(z)A \cdot A + 2K_{II}(z)A \cdot B + K_{D}(z)B \cdot B + \sqrt{\frac{2}{3}} |K_{II}(z)||A| + \sqrt{\frac{2}{3}} |K_{D}| |B| \]
\[ \leq C_2 g(\epsilon) \left( |A|^2 + |B|^2 + 1 \right). \] (36)

Furthermore, for \( X, Y = H, D \), there exists positive constants \( C_2 > C_1 > 0 \) so that
\[ C_1 g(\epsilon)|A|^2 \leq K_{XY}(\epsilon)A \cdot A \leq C_2 g(\epsilon)|A|^2, \] (37)
for all \( A \in Sym_0(3) \). Finally there exists positive constants \( C > 0 \) so that
\[ |K_{A}(\epsilon)| \leq C g(\epsilon) \] (38)
for \( X = H, D \).

**Remark 2.7.** Loosely speaking, these estimates say that the symmetric parts of the interaction energies are all comparable and give rise to a positive definite bilinear form. The fact that the same function can estimate above and below is indicative of the fact that at a fixed separation \( \epsilon \), the interaction energy cannot vary too wildly as the relative orientations of particles vary. We note that the estimates (37) and (38) are consistent with London dispersion forces for the achiral contributions [22] and the van der Meer expression for chiral contributions [33], if the interaction is 'cut-off' at close distance, a technique employed in the derivation of the Maier–Saupe free energy and evocative of the representation of such interactions as being long-range in character [23]. In fact this cut-off is necessary, as the London dispersion forces and van der Meer expression have non-integrable singularities at the origin. The non-integrability would provide significant mathematical complications. Furthermore as both are derived as leading order contributions to the interaction energy at large molecular separation, considering such interactions in the short-range would be an inappropriate use of the formulae.

Next we introduce some notation as in [32].

**Definition 2.8.** Let \( u \in L^1(\mathbb{R}^3) \), \( \epsilon > 0 \). Then define \( u^\epsilon \in L^1(\mathbb{T}^3) \) by
\[ u^\epsilon(x) = \frac{1}{\epsilon} \sum_{k \in \mathbb{Z}^3} u \left( \frac{x + 2\pi k}{\epsilon} \right). \] (39)

This definition can be interpreted in a duality-like fashion, as it is equivalent to the statement that
\[ \frac{1}{\epsilon} \int_{\mathbb{R}^3} v(x) u^\epsilon \left( \frac{x}{\epsilon} \right) \, dx = \int_{\mathbb{T}^3} u^\epsilon(x) v(x) \, dx \] (40)
for all \( v \in L^\infty(\mathbb{R}^3) \) which are \( 2\pi \)-periodic in the coordinate directions, or equivalently \( v \in L^\infty(\mathbb{T}^3) \).

Thus we can write the energy as
\[ F_\epsilon(Q, \xi) = \int_{\mathbb{T}^3} \frac{1}{\epsilon} \partial_\nu \psi(Q) + \frac{1}{\epsilon} \partial_\nu \psi(\xi) \, dx \]
\[ - \frac{1}{\epsilon^2} \int_{\mathbb{T}^3} \int_{\mathbb{T}^3} K_{III}^\epsilon(x-y) \partial_\nu \psi(Q(x) \cdot Q(y)) + 2\rho_\epsilon K_{III}^\epsilon(x-y) \partial_\nu \psi(Q(x) \cdot \xi(y) + \rho_\epsilon^2 K_{III}^\epsilon(x-y) \xi(x) \cdot \xi(y) \, dy \, dx \]
\[ - \frac{1}{\epsilon^2} \int_{\mathbb{T}^3} \int_{\mathbb{T}^3} \rho_\epsilon K_{III}^\epsilon(x-y) \xi(x) \cdot Q(y) + \frac{1}{\epsilon} \rho_\epsilon K_{III}^\epsilon(x-y) \xi(x) \cdot \xi(y) \, dy \, dx. \] (41)

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The natural function spaces for $Q, \xi$ are $L^\infty(T^3, \mathcal{U})$, as the constraints $\text{Tr}(Q) = 0$ and $\lambda_{\min}(Q) > -\frac{1}{2}$ imply $||Q||_\infty < \frac{1}{2}$ and $||\xi||_\infty < \frac{1}{2}$.

2.5. Re-writing the energy

We now turn to writing the given energy in a form more convenient for our analysis.

For the achiral terms involving the operators $K_{XY}$, we note the general identity for any symmetric bilinear form and vectors $A(x), A(y), B(x), B(y)$

$$\langle A(x) - A(y), B(x) - B(y) \rangle = \langle A(x), B(x) \rangle + \langle A(y), B(y) \rangle - 2\langle A(x), B(y) \rangle.$$

This implies that the achiral integral terms can be written as

$$\int_{T^3} \int_{T^3} K_{XY}(x-y)A(x) \cdot B(y) \, dx \, dy = \int_{T^3} \int_{T^3} K_{XY}'(x-y)A(x) \cdot B(y) - \frac{1}{2} K_{XY}(x-y)(A(x) - A(y)) \cdot (B(x) - B(y)) \, dx \, dy$$

$$= \int_{T^3} k_{XY}^0 A \cdot B \, dx \, dy - \frac{1}{2} \int_{T^3} \int_{T^3} K_{XY}'(x-y)(A(x) - A(y)) \cdot (B(x) - B(y)) \, dy \, dx. \quad (42)$$

Here the tensor $k_{XY}^0$ is defined by

$$k_{XY}^0 = \int_{T^3} K_{XY}'(z) \, dz = \int_{R^3} K_{XY}(z) \, dz. \quad (44)$$

In fact, by the symmetry properties of $K_{XY}$, we have that $k_{XY}^0$ defines a multiple of the identity operator on $\text{Sym}_0(3)$ [32, corollary 4.1]. In particular, we will abuse notation and frequently write $k_{XY}^0 A \cdot B = k_{XY}^0 (A \cdot B)$, viewing $k_{XY}^0$ as a scalar. Turning to the chiral terms $K_{\chi}$, we may write

$$\int_{T^3} \int_{T^3} K_{\chi}'(x-y)A(x) \cdot B(y) \, dx \, dy = \int_{T^3} \int_{T^3} K_{\chi}'(x-y)(A(x) - A(y)) \cdot B(y) + K_{\chi}'(x-y)A(y) \cdot B(y) \, dx \, dy$$

$$= \int_{T^3} \int_{T^3} K_{\chi}'(x-y)(A(x) - A(y)) \cdot B(y) \, dy \, dx + \int_{T^3} \left( \int_{T^3} K_{\chi}'(x-y) \, dx \right) A(y) \cdot B(y) \, dy$$

$$= \int_{T^3} \int_{T^3} K_{\chi}'(x-y)(A(x) - A(y)) \cdot B(y) \, dy \, dx. \quad (45)$$

The last equality follows from the antisymmetry of $K_{\chi}$, so that

$$\int_{T^3} K_{\chi}'(z) \, dz = - \int_{T^3} K_{\chi}'(-z) \, dz = 0. \quad (46)$$

Throughout we will use the notation that $A^{\otimes 2} = A \otimes A$ for a tensor $A$, so if $A$ lives in an inner product space $V$, and $T$ is an operator from $V$ to itself, $T \cdot A^{\otimes 2} = TA \cdot A$. Generally, for any two tensors of equal rank, $\cdot$ will denote their inner product.

We now define the functional which we will consider for periodic boundary conditions.

**Definition 2.9.** Let $\mathcal{F}_\chi : L^\infty(T^3; \mathcal{U})^2 \rightarrow \mathbb{R} \cup \{ +\infty \}$ be defined by
\[ F_\epsilon(Q, \xi) = \int_{T^3} \frac{1}{\epsilon^2} \left( \psi_\epsilon(Q) - \frac{k_{HH}^0}{2} |Q|^2 \right) + \frac{1}{\epsilon^2} \rho_0 \psi_\epsilon(\xi) - \frac{\rho_0 k_{HH}^0}{\epsilon} \cdot \xi - \frac{\rho_0^2 k_{HH}^0}{2} |\xi|^2 - c_\epsilon \, dx \]

Similarly, for the chiral terms, we expect

\[ L_{XY} = \frac{1}{2} \int_{\mathbb{R}^3} K_{XY}(z) \otimes z \otimes z \, dz. \]

for an appropriate operator \( L_{XY} \), given as an integral

\[ L_{XY} = \frac{1}{2} \int_{\mathbb{R}^3} K_{XY}(z) \otimes z \otimes z \, dz. \]
\[
\frac{1}{\epsilon} \int_{T^3} \int_{T^3} K_{xX}(x-y) A(x) \cdot (B(x) - B(y)) \, dy \, dx \\
= \int_{T^3} \int_{\mathbb{R}^3} \frac{1}{\epsilon} K_{xX} \left( \frac{x-y}{\epsilon} \right) A(x) \cdot (B(x) - B(y)) \, dy \, dx \\
= \frac{1}{\epsilon} \int_{T^3} \int_{\mathbb{R}^3} K_{xX} (z) A(x) \cdot (B(x) - B(x + cz)) \, dz \, dx \\
\approx - \int_{T^3} \int_{\mathbb{R}^3} |z|^2 K_{xX} (z) A(x) \cdot (\hat{z} \cdot \nabla) B(x) \, dz \, dx \\
= \int_{T^3} V_{xX} A(x) \cdot \nabla B(x) \, dx,
\]

where the operator
\[
V_{xX} = - \int_{\mathbb{R}^3} K_{xX}(z) \otimes z \, dz.
\]

Then, we may substitute these gradient approximations into the energy, to give
\[
F_\epsilon(Q, \xi) \approx \int_{T^3} \frac{1}{\epsilon^2} \left( \psi_s(Q(x)) - \frac{k_{BD}}{2} |Q(x)|^2 \right) + \frac{\rho_0}{\epsilon} \left( \psi_s(\xi(x)) - k_{BD}^0 Q(x) \cdot \xi(x) \right) \, dx \\
+ \frac{1}{2} \int_{T^3} L_{BD} \nabla Q(x) \cdot \nabla Q(x) - \rho_0 V_{BD} \xi(x) \cdot \nabla Q(x) - \frac{k_{BD}^0 \rho_0^2}{2} |\xi(x)|^2 \, dx \\
+ \epsilon \int_{T^3} \rho_0 L_{BD} \nabla \xi(x) \cdot \nabla \xi(x) \, dx \\
+ \epsilon^2 \int_{T^3} \frac{\rho_0^2}{2} L_{BD} \xi(x) \cdot \nabla \xi(x) \, dx.
\]

We discard all terms of order \( \epsilon \) and \( \epsilon^2 \). The leading order term, of order \( \frac{1}{\epsilon^2} \), is the bulk energy of \( Q, \psi_s(Q) - \frac{k_{BD}}{2} |Q|^2 \). As this is leading order, we assume our solutions are well approximated by restricting \( Q \) to be in the minimising set of this bulk energy, so we take \( Q = s_0 \{ n \otimes n - \frac{1}{2} I \} \) for an appropriate constant \( s_0 \) and \( n : T^3 \rightarrow S^2 \), as per proposition 2.4.

At the next order, we have a bulk-type energy for the dopant, \( \psi_s(\xi(x)) - k_{BD}^0 \xi(x) \cdot Q \). We assume this too must be well approximated by restricting \( \xi \) to the minimising set of this energy. As \( Q \) is prescribed, by symmetry and convexity arguments we can show that \( \xi(x) = \frac{s_0}{s} Q(x) \) for some constant \( s \). There is a precise explanation of the symmetry arguments available in theorem 4.11.

Now, we substitute these assumptions into the energy, and obtain that
\[
F_\epsilon \left( Q, \frac{s}{s_0} Q \right) \approx \int_{T^3} \frac{1}{2} L_{BD} \nabla Q(x) \cdot \nabla Q(x) + \frac{s_0}{s_0} \rho_0 V_{BD} Q(x) \cdot \nabla Q(x) \, dx + c_0
\]

By further symmetry arguments (see section 5), if \( n \in W^{1,2}(T^3, S^2) \), we can re-write this energy as
\[
F_\epsilon \left( Q, \frac{s}{s_0} Q \right) \approx \frac{s_0^2}{2} \int_{T^3} K_{11} (\nabla \cdot n(x))^2 + K_{22} (n(x) \cdot \nabla \times n(x) + q)^2 + K_{33} |n(x) \times \nabla \times n(x)|^2 \, dx,
\]

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where $K_{11}, K_{22}, K_{33}$ are constants relating to the energy penalisation for splay, twist and bend (respectively) of $n$. $q$ is a pseudo-scalar which dictates the tendency to twist. If $q = 0$, the ground state is given by configurations constant in space. When $q \neq 0$, the ground state is a helical structure with pitch $\frac{2 \pi}{q}$.

This formal argument bears similarities to that posed by Osipov and Kuball [29], who provide an expression for HTP through similar dispersion energies and a gradient expansion. The most significant development of this work from theirs is that in this work we prove various statements taken as ansatzes or assumptions in theirs, such as the host $Q$-tensor being uniaxial with fixed order parameter, negligibility of dopant–dopant interactions, host–dopant alignment and the applicability of a (weak)-gradient theory. In order to bypass making these assumptions we take a simpler constitutive equation on the interaction energies and a scaling limit, under which they may be proven. As the models are different the results cannot be fully consistent, however the results we obtain here are qualitatively consistent with theirs.

**Remark 3.1.** This formal argument provides insight to some of the more qualitative features of the model. Firstly, we see that all dopant–dopant interactions do not contribute to the limiting energy. Similarly, we see no change to the Frank constants themselves, nor the equilibrium order parameter of the $Q$-tensor compared to if we have a pure host system. These results are of course artifacts of the dilute regime we consider, and this formal analysis suggests there are order $\epsilon$ corrections to the Frank constants depending on the host–dopant interactions, an order $\epsilon^2$ correction to the intrinsic twist $q$ depending on the dopant–dopant chiral interaction, and order $\epsilon^2$ corrections to the Frank constants from the dopant–dopant interactions. Further corrections should be expected for $\epsilon > 0$ as the order parameters may move away from the bulk minimisers to relax elastic contributions to the energy. We will not focus on these corrections within this work, and proceed to obtain the relationship (56) in a rigorous sense.

4. $\Gamma$-convergence

4.1. Preliminary results

The estimates in assumption 2.6 translate into estimates on the non-local part of the energy, in the form

$$
C_1 \int_{\mathbb{T}^3} \int_{\mathbb{T}^3} g'(x-y) \left( \frac{|Q(x) - Q(y)|^2}{\epsilon^2} + \rho_0^2 |\xi(x) - \xi(y)|^2 - 1 \right) \, dy \, dx \\
\leq \frac{1}{4\epsilon^2} \int_{\mathbb{T}^3} \int_{\mathbb{T}^3} K_{11}^h(x-y)(Q(x) - Q(y))^2 + \rho_0^2 \epsilon^2 K_{11}^\nu(x-y)(\xi(x) - \xi(y))^2 \, dy \, dx \\
+ \frac{\rho_0}{2\epsilon} \int_{\mathbb{T}^3} \int_{\mathbb{T}^3} K_{11}^h(x-y)(Q(x) - Q(y)) \cdot (\xi(x) - \xi(y)) \, dy \, dx \\
- \frac{1}{\epsilon^2} \int_{\mathbb{T}^3} \int_{\mathbb{T}^3} \rho_0 \epsilon K_{11}^\nu(x-y)(x-y)(Q(x) - Q(y)) + \rho_0^2 \epsilon^2 K_{11}^\nu(x-y)(\xi(x) - \xi(y)) \cdot \xi(y) \, dy \, dx \\
\leq C_2 \int_{\mathbb{T}^3} \int_{\mathbb{T}^3} g'(x-y) \left( \frac{|Q(x) - Q(y)|^2}{\epsilon^2} \right) \, dy \, dx.
$$

(57)

This gives an estimate which will be exploited throughout much of this work.

**Proposition 4.1.** Let $Q, \xi \in \ell^\infty(\mathbb{T}^3, \mathbb{C})$. Then there exists a constant $C > 0$, independent of $\epsilon$, so that

$$
\int_{\mathbb{T}^3} \int_{\mathbb{T}^3} g'(x-y) \frac{|Q(x) - Q(y)|^2}{\epsilon^2} \, dx \, dy \leq C (\mathcal{F}_\epsilon(Q, \xi) + 1).
$$

(58)
Proof. First we note that
\[
\int_{T^3} \int_{T^3} g'(x-y) \left( \frac{|Q(x) - Q(y)|^2}{e^2} + \rho_0^2 |\xi(x) - \xi(y)|^2 - 1 \right) \, dy \, dx
\]
\[
\geq \int_{T^3} \int_{T^3} g'(x-y) \frac{|Q(x) - Q(y)|^2}{e^2} \, dy \, dx - \int_{T^3} \int_{T^3} g'(x-y) \left( 2\rho_0^2 |\xi|^2_{\infty} + 1 \right) \, dy \, dx
\]
\[
= \int_{T^3} \int_{T^3} g'(x-y) \frac{|Q(x) - Q(y)|^2}{e^2} \, dy \, dx - |T^3||g'||_1 \left( 2\rho_0^2 |\xi|^2_{\infty} + 1 \right).
\]
Thus using that \( \xi \) admits uniform \( L^\infty \) bounds and \( ||g'||_1 = ||g'||_1 \), which is independent of \( \epsilon \), we have that there exists a constant \( C_3 \), independent of \( \epsilon \), so that
\[
\int_{T^3} \int_{T^3} g'(x-y) \frac{|Q(x) - Q(y)|^2}{e^2} \, dy \, dx \leq \int_{T^3} \int_{T^3} g'(x-y) \left( \frac{|Q(x) - Q(y)|^2}{e^2} + \rho_0^2 |\xi(x) - \xi(y)|^2 - 1 \right) \, dy \, dx + C_3.
\]
(59)

Given that the ‘bulk energy’ integral is bounded from below by zero (following the definition of \( c_4 \) in (48)), combined with the bound in (57) for the non-local terms, and the \( L^\infty \) bounds on \( \xi \), we may write that
\[
\int_{T^3} \frac{1}{e^2} \left( \psi_s(Q) - \frac{k_{H^0}}{2} |Q|^2 \right) + \frac{\rho_0}{e} \psi_s(\xi) - \frac{\rho_0^2}{2} k_{H^0} |\xi|^2 - c_4 \, dx
\]
\[
\geq \int_{T^3} -\frac{\rho_0^2 k_{H^0}}{2} |\xi|^2 \, dx
\]
\[
\geq -\frac{\rho_0^2 k_{H^0}}{2} |T^3||\xi||_{\infty} \geq -C_4.
\]
(61)

We may combine this with the estimates in (57) and (60) to bound the non-local terms to give the final estimate that
\[
\int_{T^3} \int_{T^3} g'(x-y) \frac{|Q(x) - Q(y)|^2}{e^2} \, dy \, dx \leq \frac{1}{C_1} (F_c(Q, \xi) + C_3 + C_4).
\]
(62)

Taking \( C = \max(C_1^{-1}, C_3 + C_4) \) gives the required estimate. \( \square \)

We recall some compactness and continuity results from [32].

**Proposition 4.2 (Corollary 2.1, [32]).** Let \( A_\epsilon \in L^\infty(\mathbb{T}^3, \mathbb{Q}) \) be so that there exists some \( M \in \mathbb{R} \) with
\[
\frac{1}{e^2} \int_{T^3} \int_{T^3} g'(z) |A_\epsilon(x) - A_\epsilon(y)|^2 \, dx \, dy < M
\]
(63)
for all \( \epsilon > 0 \). Then there exists some sequence \( \epsilon_j \to 0 \) and \( A \in W^{1,2}(\mathbb{T}^3, \mathbb{Q}) \) so that \( A_{\epsilon_j} \to A \) in \( L^2 \).

**Proposition 4.3 (Proposition 2.5, [32]).** Let \( K \) satisfy the estimates in assumption 2.6. If \( \epsilon_j \to 0 \), \( A_{\epsilon_j} \in L^\infty(\mathbb{T}^3, \mathbb{Q}) \) converge in \( L^2 \) to some \( A \in W^{1,2}(\mathbb{T}^3, \mathbb{Q}) \), then
\[ \lim_{j \to \infty} \int_{T^3} \int_{T^3} 1 \epsilon K^\epsilon(x - y) (A(x) - A(y)) \otimes 2 \, dy \, dx \geq \int_{T^3} L \nabla A(x) \cdot \nabla A(x) \, dx, \]  
where

\[ L \nabla A \cdot \nabla A = \int_{\mathbb{R}^3} K(z) \frac{\partial A}{\partial x_\alpha} \cdot \frac{\partial A}{\partial x_\beta} z_\alpha z_\beta \, dz. \]  

(64)

\[ \lim_{j \to \infty} \int_{T^3} \int_{T^3} 1 \epsilon K^\epsilon(x - y) (A(x) - A(y)) \otimes 2 \, dy \, dx = \int_{T^3} L \nabla A(x) \cdot \nabla A(x) \, dx, \]  
where

\[ L \nabla A \cdot \nabla A = \int_{\mathbb{R}^3} K(z) \frac{\partial A}{\partial x_\alpha} \cdot \frac{\partial A}{\partial x_\beta} z_\alpha z_\beta \, dz. \]  

(65)

Proposition 4.4 (Proposition 2.4, [32]). Let \( K \) satisfy the estimates in assumption 2.6. If \( \epsilon_j \to 0 \), \( A_{\epsilon_j} \in W^{1,2}(T^3, \mathbb{Q}) \) converge strongly in \( W^{1,2} \) to some \( A \), then

\[ \lim_{j \to \infty} \int_{T^3} \int_{T^3} 1 \epsilon K^\epsilon(x - y) (A(x) - A(y)) \otimes 2 \, dy \, dx = \int_{T^3} L \nabla A(x) \cdot \nabla A(x) \, dx, \]  

(66)

where

\[ L \nabla A \cdot \nabla A = \int_{\mathbb{R}^3} K(z) \frac{\partial A}{\partial x_\alpha} \cdot \frac{\partial A}{\partial x_\beta} z_\alpha z_\beta \, dz. \]  

(67)

Furthermore, we recall the definition of \( \Gamma \)-convergence [6], in a simplified form relevant for this work.

Definition 4.5 (Definition 1.5, [6]). Let \( F_\epsilon : V \to \mathbb{R} \cup \{+\infty\} \), with \( V \) a normed vector space. Then we say that \( F_\epsilon \) \( \Gamma \)-converges to \( F : V \to \mathbb{R} \cup \{+\infty\} \) if the following hold:

- (Liminf inequality): For every sequence \( v_\epsilon \to v \), \( \liminf_{\epsilon \to 0} F_\epsilon(v_\epsilon) \geq F(v) \).
- (Limsup inequality): For every \( v \in V \), there exists a sequence \( v_\epsilon \to v \) with \( \lim_{\epsilon \to 0} F_\epsilon(v_\epsilon) = F(v) \).

Furthermore, if we have \( \Gamma \)-convergence and a coercivity property, then we may obtain the fundamental theorem of \( \Gamma \)-convergence, which motivates its definition.

Proposition 4.6 (Theorem 1.21, [6]). Assume that \( F_\epsilon \) \( \Gamma \)-converges to \( F \). Furthermore, assume that \( F_\epsilon \) is equicoercive, in the sense that if \( F_\epsilon(v_\epsilon) \) is uniformly bounded for a sequence \( (v_\epsilon)_{\epsilon > 0} \), there exists a subsequence \( v_j = v_{\epsilon_j} \) and \( v \in V \) so that \( v_j \to v \). Then

1. \( \lim_{\epsilon \to 0} \inf_V F_\epsilon = \min_V F \).
2. If \( v_\epsilon \) is a sequence of approximate minimisers, so that \( F_\epsilon(v_\epsilon) - \inf_V F_\epsilon \to 0 \), then there exists a subsequence \( v_j = v_{\epsilon_j} \) and \( v \) with \( F(v) = \min_V F \) so that \( v_j \to v \).

In particular, minimisers of \( F \) exist, and minimisers of \( F_\epsilon \) converge, up to subsequences, to minimisers of \( F \).

In essence, this result justifies the interpretation that \( \Gamma \)-convergence is an appropriate method of convergence for minimisation problems. In this section, we proceed to show the equicoercivity property (section 4.2), the liminf inequality (section 4.3) and limsup inequality (section 4.4).
4.2. Compactness

**Definition 4.7.** Let $\mathcal{M}$ define the minimising set of the bulk energy for the host Q-tensor in the absence of dopant. Explicitly,

$$\mathcal{M} = \left\{ Q \in \mathcal{Q} : \psi_s(Q) - \frac{k_{DH}}{2} |Q|^2 = \min_{\tilde{Q}} \psi_s(\tilde{Q}) - \frac{k_{DH}}{2} |\tilde{Q}|^2 \right\} .$$  \hfill (68)

Furthermore, we define

$$c_0 = \min_{\tilde{Q}} \psi_s(\tilde{Q}) - \frac{k_{DH}}{2} |\tilde{Q}|^2 .$$  \hfill (69)

**Assumption 4.8.** We take $k_{DH}$ sufficiently large so that

$$\mathcal{M} = \left\{ s_0 \sigma(n) : n \in S^2 \right\} ,$$  \hfill (70)

where $s_0 > 0$ is dependent on $k_{DH}$ (recall this is possible by proposition 2.4-6).

**Proposition 4.9.** Let $Q_\epsilon, \xi_\epsilon \in L^\infty(T^3, \mathcal{Q})$. If $F_\epsilon(Q_\epsilon, \xi_\epsilon)$ is uniformly bounded, then there exists some subsequence $\epsilon_j \to 0$ and $Q \in W^{1,2}(T^3, \mathcal{Q})$ so that

$$Q_\epsilon L^2 \to Q .$$

**Proof.** The coercivity estimate (57) implies that if $F_\epsilon(Q_\epsilon, \xi_\epsilon)$ is bounded, then

$$\frac{1}{\epsilon^2} \int_{T^3} \int_{T^3} g^\epsilon(x-y)|Q_\epsilon(x) - Q_\epsilon(y)|^2 \, dx \, dy$$

is bounded by proposition 4.1, so by proposition 4.2, we have compactness.

**Proposition 4.10.** Let $Q_\epsilon, \xi_\epsilon \in L^\infty(T^3, \mathcal{Q})$. If $F_\epsilon(Q_\epsilon, \xi_\epsilon)$ is uniformly bounded, then any $L^2$ cluster point $Q$ of $(Q_\epsilon)_{\epsilon > 0}$ must be pointwise almost everywhere $M$ valued. Furthermore,

$$\frac{c_\epsilon \epsilon^2 - c_0}{\epsilon} \leq -\rho_0 \ln \int_{S^2} \exp (k_{DH}^0 Q_0 \cdot p) \, dp \leq \rho_0 \min_\xi \psi_s(\xi) - k_{DH}^0 Q_0 \cdot \xi ,$$

where $Q_0 \in \mathcal{M}$, $c_0$ is as in (69), and $c_\epsilon$ is as in (48).

**Proof.** To show that $Q$ is $\mathcal{M}$ valued almost everywhere it suffices to show that

$$\int_{S^2} \psi_s(Q) - \frac{k_{DH}^0}{2} |Q|^2 - c_0 \, dx \to 0$$

with $c_0$ as in (69), as we may take a pointwise a.e. converging subsequence and apply Fatou’s lemma. To see this, first we estimate $c_\epsilon$. As the map $\xi \mapsto \psi_s(\xi) - k_{DH}^0 \xi \cdot Q$ is strictly convex for fixed $Q$, we can readily describe the unique minimiser by the critical point condition, $\xi = \Lambda^{-1}(k_{DH}^0 Q)$. This gives the minimum value as

$$\min_\xi (\psi_s(\xi) - k_{DH}^0 \xi \cdot Q) = -\ln \int_{S^2} \exp (k_{DH}^0 Q_0 \cdot p) \, dp .$$

Then if $Q_0$ is a minimiser of $\psi_s(Q) - \frac{k_{DH}^0}{2} |Q|^2$,
Now we turn to the energy estimate (57), which immediately implies
\[
F_c(Q_e, \xi_e) \geq \int_{\mathbb{T}^3} \frac{1}{c_e^2} \left( \psi_e(Q_e) - \frac{k_{\text{HH}}^0}{2} |Q_e|^2 \right) + \frac{\rho_0}{c} (\psi_e(\xi_e) - k_{\text{HH}}^0 Q_e \cdot \xi_e) - c_e - C. \tag{75}
\]

This then implies that for some \( M > 0 \)
\[
M c_e^2 \geq \int_{\mathbb{T}^3} \psi_e(Q_e) - \frac{k_{\text{HH}}^0}{2} |Q_e|^2 + \rho_0 \epsilon (\psi_e(\xi_e) - k_{\text{HH}}^0 Q_e \cdot \xi_e) - c_e^2 c_e \, dx
\]
\[
\geq \int_{\mathbb{T}^3} \psi_e(Q_e) - \frac{k_{\text{HH}}^0}{2} |Q_e|^2 + \rho_0 \epsilon \min_{\xi} \left( \psi_e(\xi) - \sqrt{\frac{7}{3}} k_{\text{HH}}^0 |\xi| \right) - c_0 - C \epsilon \, dx \tag{76}
\]
\[
\Rightarrow O(\epsilon) = \int_{\mathbb{T}^3} \psi_e(Q_e) - \frac{k_{\text{HH}}^0}{2} |Q_e|^2 - c_0 \, dx.
\]

Employing Fatou’s lemma, this gives for any subsequence with \( Q_{e_j} \to Q \) for some \( Q \), that we may take a further subsequence \( Q_k = Q_{e_k} \) converging pointwise, and
\[
0 \geq \liminf_{k \to \infty} \int_{\mathbb{T}^3} \psi_e(Q_k) - \frac{k_{\text{HH}}^0}{2} |Q_k|^2 - c_0 \, dx
\]
\[
\geq \int_{\mathbb{T}^3} \psi_e(Q) - \frac{k_{\text{HH}}^0}{2} |Q|^2 - c_0 \, dx \geq 0, \tag{77}
\]

thus as the integrand \( \psi_e(Q) - \frac{k_{\text{HH}}^0}{2} |Q|^2 - c_0 \) is non-negative and integrates to zero, it must equal zero almost everywhere, hence \( Q \in \mathcal{M} \) almost everywhere following assumption 4.8.

---

**Theorem 4.11.** Let \( Q_e, \xi_e \in L^\infty(\mathbb{T}^3, \mathcal{Q}) \). If \( F_c(Q_e, \xi_e) \) is uniformly bounded, there exists some \( Q_0 \in W^{1,2}(\mathbb{T}^3, \mathcal{M}) \) and a subsequence \( Q_j = Q_{e_j}, \xi_j = \xi_{e_j} \) so that \( Q_j \to Q_0 \) in \( L^2 \), and \( \xi_j \to \frac{\epsilon_j}{\rho_0} Q_0 \) in \( L^2 \). The constant \( \sigma_0 \), satisfies
\[
\sigma_0 = \frac{3}{2} \sigma(n) \cdot \Lambda^{-1}(k_{\text{HH}}^0), \tag{78}
\]
where \( n \in S^2 \) is arbitrary.

**Proof.** First we will show that there exists a subsequence \( \xi_{e_j}, \xi_j \overset{\ast}{\to} \xi \equiv \frac{\epsilon_j}{\rho_0} Q \) in \( L^{\infty} \), then this will be used to prove estimates to show strong \( L^2 \) convergence.

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Similarly to before, we have the energy estimate (57) which tells us
\[
M \epsilon \geq \int_{\mathcal{T}^3} \frac{1}{\epsilon} \left( \psi_s(Q) - \frac{k_{II}^0}{2} |Q_{II}|^2 \right) + \rho_0 \left( \psi_s(\xi) - k_{II}^0 Q \cdot \xi \right) - \epsilon c_\epsilon \, dx
\]
\[
\geq \int_{\mathcal{T}^3} \rho_0 \left( \psi_s(\xi) - k_{II}^0 Q \cdot \xi \right) + \frac{c_0}{\epsilon} - \epsilon c_\epsilon \, dx
\]
\[
= \int_{\mathcal{T}^3} \rho_0 \left( \psi_s(\xi) - k_{II}^0 Q_0 \cdot \xi \right) + k_{II}^0 \rho_0 \xi \cdot (Q_0 - Q_s) + \frac{c_0 - \epsilon^2 c_\epsilon}{\epsilon} \, dx
\]
\[
\geq \int_{\mathcal{T}^3} \rho_0 \left( \psi_s(\xi) - k_{II}^0 Q_0 \cdot \xi \right) - \rho_0 \min_{\xi} \left( \psi_s(\xi) - k_{II}^0 Q_0 \cdot \xi \right) + k_{II}^0 \rho_0 \xi \cdot (Q_0 - Q_s) \, dx.
\]
(79)

where \( Q_0 \in L^\infty(\mathbb{T}^3, \mathcal{Q}) \) is arbitrary. Now we take a subsequence so that \( \epsilon_j \to 0, \xi_{\epsilon_j} \to \xi \) in \( L^\infty \), and \( Q_{\epsilon_j} = Q_0 \to Q \) in \( L^2 \), which is permitted as \( \|\xi\|_\infty < \frac{\epsilon}{2} \) and proposition 4.9. Furthermore, take \( Q_0 = Q \). Then
\[
0 \leq \int_{\mathcal{T}^3} \rho_0 \left( \psi_s(\xi) - k_{II}^0 Q \cdot \xi \right) - \rho_0 \min_{\xi} \left( \psi_s(\xi) - k_{II}^0 Q \cdot \xi \right) \, dx
\]
\[
\leq M \epsilon - \int_{\mathcal{T}^3} \rho_0 k_{II}^0 \xi \cdot (Q - Q_0) \, dx
\]
\[
\leq M \epsilon + \rho_0 k_{II}^0 \|\xi\|_2 \|Q - Q_0\|_2 \to 0.
\]
(80)

Now, as \( \psi_s \) is strictly convex, this yields
\[
0 = \lim_{j \to \infty} \int_{\mathcal{T}^3} \rho_0 \left( \psi_s(\xi) - k_{II}^0 Q \cdot \xi \right) - \rho_0 \min_{\xi} \left( \psi_s(\xi) - k_{II}^0 Q \cdot \xi \right) \, dx
\]
\[
\geq \int_{\mathcal{T}^3} \rho_0 \left( \psi_s(\xi) - k_{II}^0 Q \cdot \xi \right) - \rho_0 \min_{\xi} \left( \psi_s(\xi) - k_{II}^0 Q \cdot \xi \right) \, dx.
\]
(81)

This means that \( \xi \) must be pointwise in the minimum energy wells of \( \tilde{\xi} \mapsto \psi_s(\tilde{\xi}) - Q \cdot \tilde{\xi} \). This is a strictly convex function so its minimizing set must be a single point, and by taking the derivative we see that almost everywhere
\[
\xi(x) = \Lambda^{-1}(k_{II}^0 Q(x)).
\]
(82)

More so, as \( Q \) is \( \mathcal{M} \) valued almost everywhere, this means that we can write \( Q = s_0 \sigma(n) = \Lambda^{-1}(k_{II}^0 s_0 \sigma(n)) \). Since \( \Lambda^{-1} \) is frame invariant, this implies \( \xi \) is also uniaxial with director \( n \). This implies \( \xi = s_c \sigma(n) \) for some \( s_c \), which can readily be found by taking the inner product of (82) against \( \frac{\epsilon}{2} \sigma(n) \), giving
\[
s_c = \frac{3}{2} \sigma(n) \cdot (s_c \sigma(n)) = \frac{3}{2} \sigma(n) \cdot \Lambda^{-1}(k_{II}^0 s_0 \sigma(n)).
\]
(83)

Alternatively, we can write \( \xi = \frac{\epsilon}{2} Q \).

To show that \( \xi \) converges in \( L^2 \), first we note that as the second derivative of the bulk energy \( \left( \psi_s(\xi) - Q \cdot \xi \right) - \min_{\tilde{\xi}} \left( \psi_s(\tilde{\xi}) - k_{II}^0 Q \cdot \tilde{\xi} \right) \) is positive definite, and independent of \( Q \), this implies that there is some \( \delta > 0 \) so that if \( |\bar{\xi} - \xi(x)| < \delta \), then
\[
(\psi_s(\xi) - Q \cdot \xi) - \min_{\tilde{\xi}} \left( \psi_s(\tilde{\xi}) - k_{II}^0 Q \cdot \tilde{\xi} \right) \geq C|\bar{\xi} - \xi(x)|^2.
\]
The constant \( C \) can be taken
uniformly in $Q \in \mathcal{M}$. So we can estimate
\[
\|\xi_j - \xi\|_2^2 = \int_{|\xi_j - \xi| > \delta} |\xi_j(x) - \xi(x)|^2 \, dx + \int_{|\xi_j - \xi| \leq \delta} |\xi_j(x) - \xi(x)|^2 \, dx.
\] (84)

To estimate the first term, it suffices to show that the set where $|\xi_j - \xi| > \delta$ is of vanishing measure as $j \to \infty$, as $\xi_j, \xi_j$ are uniformly bounded. However, the uniform estimate on the bulk energy means that there is some constant $C_1 > 0$ with
\[
\min_{|\xi_j - \xi| > \delta} \left( \psi_j(\hat{\xi}) - Q \cdot \hat{\xi} - \kappa^{\mathrm{DH}}_Q \cdot \hat{\xi} \right) > C_1,
\] (85)
so this follows from the energy estimate.

For the second term, we estimate this as
\[
\int_{|\xi_j - \xi| \leq \delta} |\xi_j(x) - \xi(x)|^2 \, dx \leq \frac{1}{C} \int_{|\xi_j - \xi| \leq \delta} \left( \psi_j(\xi) - Q \cdot \xi - \min_{\xi} \left( \psi_j(\xi) - \kappa^{\mathrm{DH}}_Q \cdot \xi \right) \right) \, dx \to 0.
\] (86)
Combining these gives that $\|\xi_j - \xi\|_2 \to 0$.

4.3. Liminf inequality

Within this section we will proceed to show the necessary liminf inequality for our $\Gamma$-convergence result. The necessary ingredients are to show that given an energy estimate, the host–host interaction term has the asymptotic lower bound of the quadratic energy in $\nabla Q$, the chiral host–dopant term converges to the correct term linear in $\nabla Q$, and all other interaction terms converge to zero, which are strongly aided by our compactness results.

**Proposition 4.12.** Let $Q_j, \xi_j \in L^\infty(T^3, \mathbb{R})$. Assume that $\mathcal{F}^j(Q_j, \xi_j)$ is uniformly bounded. Then, we may take a subsequence $\epsilon_j \to 0$ so that for $Q_j = Q_j^e, \xi_j = \xi_j^e$,
\[
\frac{1}{\epsilon_j} \int_{T^3} \int_{T^3} \kappa^{\mathrm{DH}}_Q(x - y) \left( Q_j(x) - Q_j(y) \right) \cdot (\xi_j(x) - \xi_j(y)) \, dy \, dx \to 0.
\] (87)

**Proof.** First, we take a subsequence so that $Q_j \to Q \in L^2$; $\xi_j \to \xi = \frac{s_0}{s_0} Q$ in $L^2$. Then estimate
\[
\frac{1}{\epsilon_j} \int_{T^3} \int_{T^3} \kappa^{\mathrm{DH}}_Q(x - y) \left| (Q_j(x) - Q_j(y)) \cdot (\xi_j(x) - \xi_j(y)) \right| \, dy \, dx \leq \frac{C}{\epsilon_j} \int_{T^3} \int_{T^3} g^u(x - y) |Q_j(x) - Q_j(y)| \cdot |\xi_j(x) - \xi_j(y)| \, dy \, dx
\]
\[
= \frac{C}{\epsilon_j} \int_{T^3} \int_{T^3} g^u(x - y) |Q_j(x) - Q_j(y)| \cdot \left| \xi_j(x) - \frac{s_0 x_0}{s_0} Q_j(x) + \frac{s_0 x_0}{s_0} Q_j(x) - \frac{s_0 x_0}{s_0} Q_j(y) + \frac{s_0 x_0}{s_0} Q_j(y) - \xi_j(y) \right| \, dy \, dx
\]
\[
\leq \frac{C}{\epsilon_j} \int_{T^3} \int_{T^3} g^u(x - y) |Q_j(x) - Q_j(y)| \left( \frac{s_0}{s_0} |Q_j(x) - Q_j(y)| + \frac{s_0}{s_0} |Q_j(x) - \xi_j(x)| + \frac{s_0}{s_0} |Q_j(y) - \xi_j(y)| \right) \, dy \, dx
\]
\[
= \frac{C}{\epsilon_j} \int_{T^3} \int_{T^3} g^u(x - y) |Q_j(x) - Q_j(y)| \left( \frac{s_0}{s_0} |Q_j(x) - Q_j(y)| + 2 \left| \frac{s_0}{s_0} Q_j(x) - \xi_j(x) \right| \right) \, dy \, dx
\] (88)
we estimate the two summands in turn. For the left-hand term,
\[
\frac{C}{\epsilon j} \int_{T^T_j} \int_{T^T_j} g^\epsilon'(x - y) |Q_j(x) - Q_j(y)| \frac{2}{x_0} |Q_j(x) - Q_j(y)| \, dy \, dx \\
= \epsilon j \frac{C}{x_0} \int_{T^T_j} \int_{T^T_j} g^\epsilon'(x - y) |Q_j(x) - Q_j(y)|^2 \, dy \, dx
\]
\[
\leq C \epsilon j \left( F_j(Q_j, \xi_j) + 1 \right) \to 0
\]  

from the energy bound. For the remaining term,
\[
\frac{2C}{\epsilon j} \int_{T^T_j} \int_{T^T_j} g^\epsilon'(x - y) |Q_j(x) - Q_j(y)| \left| \frac{2}{x_0} Q_j(x) - \xi_j(x) \right| \, dy \, dx
\]
\[
\leq 2C \left( \epsilon j \right)^{\frac{1}{2}} \left( \int_{T^T_j} \int_{T^T_j} g^\epsilon'(x - y) |Q_j(x) - Q_j(y)|^2 \, dx \, dy \right)^{\frac{1}{2}} \left( \int_{T^T_j} \int_{T^T_j} \left| \frac{2}{x_0} Q_j(x) - \xi_j(x) \right|^2 \, dy \, dx \right)^{\frac{1}{2}}
\]
\[
\leq C \left( F_j(Q_j, \xi_j) + 1 \right)^{\frac{1}{2}} \left| \frac{2}{x_0} Q_j - \xi \right|_{2} \| g^\epsilon \|_2 (92)
\]

where Fubini’s theorem is used. As the energy is bounded, $g^\epsilon$ is $L^1$-bounded, and $\xi_j, \frac{2}{x_0} Q_j$ both converge to $\xi$ in $L^2$, this term also vanishes as $\epsilon \to 0$, giving the required result.

**Proposition 4.13.** Let $Q_j, \xi_j \in L^\infty(T^T_j, \mathbb{Q})$. Assume that $F_j(Q_j, \xi_j)$ is uniformly bounded. Then
\[
\lim_{\epsilon \to 0} \int_{T^T_j} \int_{T^T_j} K^{\epsilon}_i(x - y) \xi_j(x) \cdot (\xi_j(x) - \xi_j(y)) \, dy \, dx = 0.
\]

**Proof.** We estimate
\[
\left| \int_{T^T_j} \int_{T^T_j} K^{\epsilon}_i(x - y) \xi_j(x) \cdot (\xi_j(x) - \xi_j(y)) \, dy \, dx \right|
\]
\[
\leq C \epsilon \int_{T^T_j} \int_{T^T_j} g^\epsilon(x - y) |\xi_j(x) - \xi_j(y)| \, dx \, dy
\]
\[
\leq C \epsilon \left( \int_{T^T_j} \int_{T^T_j} g^\epsilon(x - y) |\xi_j(x) - \xi_j(y)|^2 \, dx \, dy \right)^{\frac{1}{2}} \left( \int_{T^T_j} \int_{T^T_j} g^\epsilon(x - y) \, dx \, dy \right)^{\frac{1}{2}}
\]
\[
= C \epsilon \| g^\epsilon \|_2^2 \left( \int_{T^T_j} \int_{T^T_j} g^\epsilon(x - y) |\xi_j(x) - \xi_j(y)|^2 \, dx \, dy \right)^{\frac{1}{2}}
\]
\[
\leq C \epsilon \| g^\epsilon \|_2^2 \left( F_j(Q_j, \xi_j) + 1 \right)^{\frac{1}{2}} = O(\epsilon)
\]  

from the energy estimate (57). 

Before proceeding with the next result we introduce some further notation for finite difference operators.
Definition 4.14. Let \( u : \mathbb{R}^3 \to V \) for a vector space \( V \). Let \( z \in \mathbb{R}^3 \). Define the finite difference \( D_z u : \mathbb{R}^3 \to V \) by

\[
D_z u(x) = \frac{1}{|z|} (u(x + z) - u(x)).
\]

(93)

Proposition 4.15. Assume that \( Q_j, \xi_j \) converge in \( L^2 \) to \( Q, \xi \in W^{1,2}(\mathbb{T}^3, \mathcal{Q}) \) with \( \mathcal{F}(Q, \xi) < M \). Then we have a subsequence \( j \to 0 \), so that for \( Q_j = Q, \xi_j = \xi \),

\[
\frac{1}{\epsilon_j} \int_{\mathbb{T}^3} \int_{\mathbb{T}^3} K^\epsilon_H(x-y) \xi_j(x) \cdot (Q_j(x) - Q_j(y)) \, dx \, dy \to \int_{\mathbb{T}^3} \xi(x) \cdot \left( \int_{\mathbb{R}^3} K_H(z) \otimes z \, dz \right) \cdot \nabla Q(x) \, dx.
\]

(94)

Proof. First, we define \( u_j(x) = \frac{1}{\epsilon_j} \int_{\mathbb{T}^3} K^\epsilon_H(x-y)(Q_j(x) - Q_j(y)) \, dy \). The strategy is first to obtain a uniform \( L^2 \) bound on \( u_j \) so that we may take a weakly converging subsequence, and then the limit can be identified by investigating the limit in the sense of distributions. We estimate

\[
\|u_j\|^2 \leq C \int_{\mathbb{T}^3} \left( \int_{\mathbb{T}^3} g^\epsilon(x-y) |Q_j(x) - Q_j(y)| \, dy \right)^2 \, dx
\]

\[
\leq C \int_{\mathbb{T}^3} \left( \int_{\mathbb{T}^3} g^\epsilon(x-y)|Q_j(x) - Q_j(y)| \, dy \right)^2 \, dx
\]

\[
\leq C \int_{\mathbb{T}^3} \int_{\mathbb{T}^3} g^\epsilon(x-y)(Q_j(x) - Q_j(y))^2 \, dy \, dx
\]

\[
\leq C \int_{\mathbb{T}^3} \int_{\mathbb{T}^3} g^\epsilon(x-y)(Q_j(x) - Q_j(y))^2 \, dy \, dx
\]

\[
\leq C \left( \mathcal{F}(Q, \xi) + 1 \right).
\]

So this implies that \( u_j \) is \( L^2 \) bounded. Hence we can take a subsequence \( \epsilon_j \) with \( Q_j \to Q \in W^{1,2}(\mathbb{T}^3, \mathcal{M}) \) and \( Q_j(x) \to Q(x) \) pointwise almost everywhere, \( \xi_j = \xi \), and \( u_j \to u \). We find \( u \) by integrating against a test function \( \phi \in \mathcal{D}(\mathbb{T}^3) \). This gives, by a change of variables \( z = x - y \),

\[
\int_{\mathbb{T}^3} u_j(x) \phi(x) \, dx = \frac{1}{\epsilon_j} \int_{\mathbb{T}^3} \int_{\mathbb{T}^3} \phi(x) K^\epsilon_H(x-y)(Q_j(x) - Q_j(y)) \, dy \, dx
\]

\[
= -\frac{1}{\epsilon_j} \int_{\mathbb{T}^3} \int_{\mathbb{T}^3} \phi(x) K^\epsilon_H(z)(z) D_{-z} Q_j(x) \, dz \, dx
\]

\[
= -\frac{1}{\epsilon_j} \int_{\mathbb{T}^3} K^\epsilon_H(z)(z) \int_{\mathbb{T}^3} \phi(x) D_{-z} Q_j(x) \, dx \, dz
\]

\[
= -\frac{1}{\epsilon_j} \int_{\mathbb{T}^3} K^\epsilon_H(z)(z) \int_{\mathbb{T}^3} D_z \phi(x) Q_j(x) \, dx \, dz.
\]

(96)

Now, as \( \phi \) is smooth and periodic,

\[
\frac{1}{\epsilon_j} \int_{\mathbb{T}^3} \int_{\mathbb{T}^3} K^\epsilon_H(z) Q_j(x) |z| D_z \phi(x) \, dx \, dz = \int_{\mathbb{T}^3} \int_{\mathbb{R}^3} K_H(z) Q_j(x) |z| D_z \phi(x) \, dx \, dz.
\]

(97)
The integrand can be bounded by $Cg(z)|z||\nabla \phi|_\infty$ pointwise almost everywhere, which, as $g \in L^1$ with finite second moment and $\mathbb{T}^3$ is bounded, is integrable over $(x,z) \in \mathbb{T}^3 \times \mathbb{R}^3$. Furthermore, as $\phi$ is smooth, $D_{x,z}\phi(x) \to (\hat{z} \cdot \nabla)\phi(x)$. Recalling $Q_j(x)$ converges pointwise almost everywhere to $Q(x)$ also, this implies that the integrand converges pointwise to $K_{cH}(z)Q(x)(z \cdot \nabla)\phi(x)$ as $\epsilon_j \to 0$. Thus by dominated convergence,

$$
\lim_{j \to \infty} -\frac{1}{\epsilon_j} \int_{\mathbb{T}^3} K'_{cH}(z)|z| \int_{\mathbb{T}^3} D_{x} \phi(x)Q_j(x) \, dx \, dz \\
= -\int_{\mathbb{T}^3} \int_{\mathbb{R}^3} K_{cH}(z)Q(x)(z \cdot \nabla)\phi(x) \, dz \, dx \\
= \int_{\mathbb{T}^3} \left( \int_{\mathbb{R}^3} K_{cH}(z) \odot z \, dz \right) \cdot \nabla Q(x)\phi(x) \, dx.
$$

(98)

As the limit in $D'(\mathbb{T}^3)$ and weak limit in $L^2$ must coincide,

$$
u = \left( \int_{\mathbb{R}^3} K_{cH}(z) \odot z \, dz \right) \cdot \nabla Q. \quad (99)
$$

Now, finally, we note that

$$
\frac{1}{\epsilon_j} \int_{\mathbb{T}^3} \int_{\mathbb{T}^3} K'_{cH}(x-y)\xi_j(x) \cdot (Q_j(x) - Q_j(y)) \, dx \, dy \\
= \int_{\mathbb{T}^3} \xi_j(x) \cdot u_j(x) \, dx \\
\to \int_{\mathbb{T}^3} \xi(x) \cdot u(x) \, dx \\
= \int_{\mathbb{T}^3} \xi(x) \cdot \left( \int_{\mathbb{R}^3} K_{cH}(z) \odot z \, dz \right) \cdot \nabla Q(x) \, dx,
$$

(100)

as $\xi_j$ converges in $L^2$ strongly.

**Theorem 4.16.** Let $Q \in W^{1,2}(\mathbb{T}^3, \mathcal{M})$, $Q_\epsilon \rightharpoonup Q$, $\xi_\epsilon \rightharpoonup_{L^2} \xi_0$. Then

$$
\liminf_{\epsilon \to 0} \mathcal{F}_\epsilon(Q_\epsilon, \xi_\epsilon) \geq \int_{\mathbb{T}^3} \frac{1}{2} \nabla Q \cdot \nabla Q - \frac{s_v \rho_0}{s_0} V Q \cdot \nabla Q \, dx - \frac{s_v^2 \rho_0^2 \kappa_0}{3} |\Omega|.
$$

(101)

Here $L, V$ are given as

$$
L \nabla Q \cdot \nabla Q = \frac{1}{2} \left( \int_{\mathbb{R}^3} K_{HI}(z)_{\alpha \beta} \, dz \right) \frac{\partial Q}{\partial x_\alpha} \cdot \frac{\partial Q}{\partial x_\beta},
$$

$$
V Q \cdot \nabla Q = \left( \int_{\mathbb{R}^3} K_{cH}(z)_{\alpha} \, dz \right) Q \cdot \frac{\partial Q}{\partial x_\alpha}.
$$

(102)

**Proof.** We assume the liminf is finite, else there is nothing to prove. By observing many of the terms in the energy are non-negative, we have for any $Q_\epsilon, \xi_\epsilon$
\[ F_{\epsilon}(Q, \xi) \geq \frac{1}{\epsilon^2} \int_{T^3} \int_{T^3} \frac{1}{4} K_{\text{inh}}(x-y) (Q_\epsilon(x) - Q_\epsilon(y))^2 - \rho_0 K_{\text{inh}}^\epsilon(x-y) \xi_\epsilon(x) \cdot (Q_\epsilon(x) - Q_\epsilon(y)) \]
\[ + \frac{1}{2} \rho_0 K_{\text{inl}}^\epsilon(x-y) (Q_\epsilon(x) - Q_\epsilon(y)) \cdot (\xi_\epsilon(x) - \xi_\epsilon(y)) - \rho_0^\epsilon \xi F Q \to \cdot \nabla \xi \]
\[ - \frac{\rho_0^\epsilon |\xi|^2}{2}. \quad (103) \]

We may take a subsequence \( \epsilon_j \to 0 \) with \( Q_j \to Q \in W^{1,2}(T^3; \mathcal{M}) \) strongly in \( L^2 \) and \( \xi_j = \xi_{\epsilon_j} \to \frac{\xi}{\alpha_0} Q \) strongly in \( L^2 \) such that \( \liminf_{\epsilon \to 0} F(Q_\epsilon, \xi_\epsilon) - \lim_{j \to \infty} F_j(Q_j, \xi_j) \). From propositions 4.12 and 4.13, we see that the second line terms vanish as \( \epsilon \to 0 \). Then as \( \xi_j \to \frac{\xi}{\alpha_0} Q \) strongly in \( L^2 \), \( \lim_{j \to \infty} ||\xi_j||_2 = \frac{\alpha_0}{\alpha_0} ||Q||_2 \). From proposition 4.15 it is seen that
\[ \int_{T^3} \int_{T^3} \rho_0 K_{\text{inl}}^\epsilon(x-y) \xi_\epsilon(x) \cdot (Q_\epsilon(x) - Q_\epsilon(y)) \, dx \, dy \to \rho_0 \int_{T^3} V \xi \cdot \nabla Q \, dx \]
\[ = \frac{s_c \rho_0}{s_0} \int_{T^3} V Q \cdot \nabla Q \, dx \quad (104) \]

and from proposition 4.3 we have that
\[ \liminf_{\epsilon \to 0} \frac{1}{4\epsilon^2} \int_{T^3} \int_{T^3} K_{\text{inh}}^\epsilon(x-y) (Q_\epsilon(x) - Q_\epsilon(y))^2 \geq \int_{T^3} \frac{1}{2} L V Q \cdot \nabla Q \, dx. \quad (105) \]

Combining these gives the required result.

\[ \square \]

### 4.4. Limsup inequality

The ‘bulk’-type contribution to the energy is singular as \( \epsilon \to 0 \), so in constructing recovery sequences it is essential we can gain strong control over the bulk energy. The simplest means to do so will be to construct recovery sequences that, for each \( \epsilon > 0 \), have zero bulk energy. As the bulk energy itself depends on \( \epsilon \) in a non-trivial way, before proceeding we must first understand the behaviour of the minimisers of the bulk energy. The perturbative nature of the \( \epsilon \) dependence makes this tractable however.

**Proposition 4.17.** There exists \( \epsilon^* > 0 \) so that for all \( 0 < \epsilon < \epsilon^* \), there exists minimisers of \( \psi_\epsilon(Q) - \frac{k_{\text{inh}}}{\epsilon^2} ||Q||^2 + \epsilon \rho_0 (\psi_\epsilon(\xi) - k_{\text{inl}}^0 Q \cdot \xi) \) of the form
\[ Q_\epsilon = s_0(\epsilon) \sigma(n), \]
\[ \xi_\epsilon = s_c(\epsilon) \sigma(n). \quad (106) \]

Furthermore, as \( \epsilon \to 0 \), \( s_0(\epsilon) \to s_0, s_c(\epsilon) \to s_c \).

**Proof.** Let \( \epsilon > 0 \). First, we minimise with respect to \( \xi \) in the same manner as theorem 4.11, yielding \( \Lambda(\xi) = k_{\text{inl}}^0 Q \). We substitute this back into the expression, recalling the alternative expression for \( \psi_\epsilon \), as
\[ \psi_s(\xi) - k^0_{tD}Q \cdot \xi = -\ln \int_{\mathbb{R}^3} \exp(k^0_{tD}Qp \cdot p) \, dp. \]  

(107)

Returning to our minimisation problem, we have

\[ \min_{\psi_\xi} \psi_s(Q) - \frac{k^0_{tD}}{2} |Q|^2 + \epsilon \rho_0 (\psi_s(\xi) - k^0_{tD}Q \cdot \xi) \]

\[ = \min_Q \psi_s(Q) - \frac{k^0_{tD}}{2} |Q|^2 - \epsilon \rho_0 \ln \int_{\mathbb{R}^3} \exp(k^0_{tD}Qp \cdot p) \, dp. \]  

(108)

We proceed by a perturbation argument. Define the perturbed bulk energy as

\[ \psi'_B(Q) = \psi_s(Q) - \frac{k^0_{tD}}{2} |Q|^2 - \epsilon \rho_0 \ln \int_{\mathbb{R}^3} \exp(k^0_{tD}Qp \cdot p) \, dp. \]  

(109)

The method of proof is to exploit the known uniaxiality of minimisers of \( \psi'_B \), and to exploit the implicit function theorem to show that there exists a continuous branch of uniaxial minimisers for small \( \epsilon \). Using the implicit function theorem is equivalent to showing there is no bifurcation of minimisers of \( \psi'_B \) at \( \epsilon = 0 \) and \( Q = Q_0 = s_0 \sigma(n) \).

As \( \psi'_B \) is a frame indifferent function, its minimisers are not generally isolated. This provides a small obstacle to using the implicit function theorem in a direct way. To overcome this obstacle, we only consider Q-tensors with a fixed eigenbasis. We may parametrise the space of Q-tensors with eigenbasis \( e_1, e_2, e_3 \) as \( \eta(s, t) = s \sigma(e_1) + t(e_2 \otimes e_2 - e_1 \otimes e_3) \), for \( s, t \in \mathbb{R} \). Then defining

\[ \tilde{\psi}'_B(s, t) = \psi'_B(\eta(s, t)), \]

(110)

we have exactly three isolated minimisers of \( \tilde{\psi}'_B \) given by \( (s, t) \) as \( (s_0, 0), (-\frac{s_0}{2}, \frac{s_0}{2}), (-\frac{s_0}{2}, -\frac{s_0}{2}) \). These three minimisers are all equivalent under rotations, corresponding to permutations of the eigenbasis.

As all three minimisers are equivalent, we consider the simplest, \( (s_0, 0) \). We note that \( \eta(s, t) \) and \( \eta(s, -t) \) are equivalent by symmetry, corresponding to an exchange of \( e_2, e_3 \). In particular, if there existed a branch of minimisers of \( \tilde{\psi}'_B,(s_0(\epsilon), t(\epsilon)) \) with \( t(\epsilon) \) non-zero for certain \( \epsilon \), then there must also be a corresponding branch \( (s_0(\epsilon), -t(\epsilon)) \). The consequence of this is that if we can show there is, locally, a unique branch of minimisers of \( \tilde{\psi}'_B \) as \( \epsilon \to 0 \) going through \( (s_0, 0) \) at \( \epsilon = 0 \), we must have that \( t(\epsilon) = 0 \). That is to say, minimisers on such a branch will be uniaxial.

From here, we may use the stability result of Li et al [19] (see also proposition 2.4, part 7), which states that there exists \( c_1 > 0 \) so that

\[ \frac{\partial^2}{\partial(s, t)^2} \tilde{\psi}'_B(s_0, 0)(s, t) \cdot (s, t) = \nabla^2 \eta(s_0, 0) \eta(s, t) \cdot \eta(s, t) > c_1(s^2 + t^2) \]

(111)

for all \( s, t \). Therefore as \( \tilde{\psi}'_B \) is smooth, the critical point condition on \( (s, t), \frac{\partial}{\partial(s, t)} \tilde{\psi}'_B = (0, 0) \) admits a (locally) unique, smooth branch of solutions \( (s_0(\epsilon), t(\epsilon)) \) passing through \( (s_0, 0) \), and
as explained before the uniqueness implies \( t(\epsilon) = 0 \) for \( \epsilon \) sufficiently small. Returning to the tensorial language, this means that for \( \epsilon \) sufficiently small, there exists global minimisers \( Q_\epsilon = s_\epsilon(\epsilon)\sigma(n) \), where \( s_\epsilon(\epsilon) \) is smooth at \( \epsilon = 0 \), \( s_0(0) = s_0 \), and \( n \in S^2 \) is arbitrary.

Recalling that \( \xi_\epsilon \) satisfies the equation \( \Lambda(\xi_\epsilon) = \xi_{\text{id}}(Q_\epsilon) \), we can use that \( \Lambda \) is frame indifferent to infer that the rotations with \( RQ_\epsilon R^T = \xi_\epsilon \) are precisely those with \( RQ_\epsilon R^T = Q_\epsilon \), hence \( \xi_\epsilon \) must be uniaxial with the same director as \( Q_\epsilon \), hence \( \xi_\epsilon = s_\epsilon(\epsilon)\sigma(n) \). Furthermore, as \( \Lambda \) admits a continuous inverse, and \( Q_\epsilon \to Q = s_0\sigma(n) \), this implies

\[
s_\epsilon(\epsilon)\sigma(n) = \xi_\epsilon = \Lambda^{-1}(k_{\text{id}}^0Q_\epsilon) \to \Lambda^{-1}(k_{\text{id}}^0Q_0) = \xi_0 = s_\epsilon\sigma(n).
\]  

(112)

Hence \( s_\epsilon(\epsilon) \to s_\epsilon \).

\[ \square \]

**Proposition 4.18.** Let \( Q \in W^{1,2}(T^3; \mathcal{M}) \). Let \( Q_\epsilon = \frac{s_\epsilon(\epsilon)}{s_0}Q \), \( \xi_\epsilon = \frac{s_\epsilon(\epsilon)}{s_0}Q \). Then \( Q_\epsilon \to Q \) in \( W^{1,2} \), \( \xi_\epsilon \to \frac{s_\epsilon(\epsilon)}{s_0}Q \) in \( W^{1,2} \), and

\[
\lim_{\epsilon \to 0} F_\epsilon(Q_\epsilon, \xi_\epsilon) = \int_{T^3} \frac{1}{2} L \nabla Q \cdot \nabla Q - \frac{s_\epsilon(\epsilon)}{s_0}VQ \cdot \nabla Q \, dx - \frac{s_\epsilon^2(\epsilon)^3 k_{\text{id}}^0}{3} |\Omega|,
\]

(113)

where \( L, V \) are as in (102).

**Proof.** The fact that \( Q_\epsilon, \xi_\epsilon \to Q_0, \xi_0 \) is immediate from proposition 4.17. It remains to show the energy admits the correct limit. As \( Q_\epsilon, \xi_\epsilon \) by definition have zero bulk energy, and by propositions 4.12 and 4.13, we can remove redundant terms in the energy that vanish in the limit to give

\[
\lim_{\epsilon \to 0} F_\epsilon(Q_\epsilon, \xi_\epsilon) = \lim_{\epsilon \to 0} \int_{T^3} \frac{1}{4\pi} \frac{1}{r^2} K_{\text{id}}(x-y) \cdot (Q_\epsilon(x) - Q_\epsilon(y)) \, dx - \frac{\rho_0}{2} \int_0^\infty \frac{\rho_0(x)}{2 \rho_0} |\xi_\epsilon(x)\|^2 \, dx \\
= \lim_{\epsilon \to 0} \int_{T^3} \frac{s_\epsilon(\epsilon)^2}{4\rho_0^2} K_{\text{id}}(x-y) \cdot (Q(x) - Q(y)) \, dx + \frac{\rho_0(\epsilon) s_\epsilon(\epsilon)}{2 \rho_0} K_{\text{id}}(Q(x) - Q(y)) \, dx \\
- \frac{\rho_0^2}{2} \int_0^\infty \frac{s_\epsilon(\epsilon)^2 k_{\text{id}}^0}{2 \rho_0} |Q(x)|^2 \, dx.
\]  

(114)

Now, we use the convergence result of proposition 4.4 on the first term, proposition 4.15 on the second term, and that \( s_\epsilon(\epsilon) \to s_0 \), \( s_\epsilon(\epsilon) \to s_\epsilon \), to give

\[
\lim_{\epsilon \to 0} F_\epsilon(Q_\epsilon, \xi_\epsilon) = \int_{T^3} \frac{1}{2} L \nabla Q \cdot \nabla Q - \frac{s_\epsilon(\epsilon)}{s_0}VQ \cdot \nabla Q \, dx - \frac{s_\epsilon^2(\epsilon)^3 k_{\text{id}}^0}{3} |\Omega|.
\]

(115)

\[ \square \]

This now leads us to the main result.

**Theorem 4.19.** The functionals \( F_\epsilon : L^\infty(T^3; \mathcal{Q})^2 \to \mathbb{R} \cup \{ +\infty \} \) as defined in (41) \( \Gamma \)-converge with respect to strong-\( L^2 \) convergence to the functional \( F_{\text{off}} : L^\infty(T^3; \mathcal{Q}) \to \mathbb{R} \cup \{ +\infty \} \) defined by

\[
F_{\text{off}}(Q, \xi) = \int_{T^3} \frac{1}{2} L \nabla Q \cdot \nabla Q - \frac{s_\epsilon(\epsilon)}{s_0}VQ \cdot \nabla Q \, dx - \frac{s_\epsilon^2(\epsilon)^3 k_{\text{id}}^0}{3} |\Omega|
\]

(116)

if \( Q, \xi \in W^{1,2}(T^3; \mathcal{Q})^2 \), and \( Q(x) \in \mathcal{M} \) and \( \xi(x) = \frac{s_\epsilon(\epsilon)}{s_0}Q(x) \) pointwise almost everywhere, and \( +\infty \) otherwise. The operators \( L, V \) are defined by
\[
L \nabla Q \cdot \nabla Q = \frac{1}{2} \left( \int_{\mathbb{R}^3} K_{HH}(z) z_\alpha z_\beta \, dz \right) \frac{\partial Q}{\partial x_\alpha} \cdot \frac{\partial Q}{\partial x_\beta},
\]

\[
VQ \cdot \nabla Q = \left( \int_{\mathbb{R}^3} K_{H}(z) z_\alpha \, dz \right) Q \cdot \frac{\partial Q}{\partial x_\alpha}
\]

(117)

5. Coefficients in standard form

5.1. Landau coefficients

In \( F_{OF} \), the term quadratic in \( \nabla Q \) is given by \( \frac{1}{2} L \nabla Q \cdot \nabla Q \), and is frame indifferent. This reduces the degrees of freedom of \( L \) down to three elastic constants, and by symmetry we know that any such function must be of the form

\[
L \nabla Q \cdot \nabla Q = L_1 Q_{ij} Q_{jk} + L_2 Q_{ij} Q_{jk} + L_3 Q_{ij} Q_{jk}
\]

(118)

for scalars \( L_1, L_2, L_3 \) that can be obtained by testing various configurations of \( \nabla Q \) (see e.g. [7, 25, 26]). If \( L \) were to have depended on \( Q \), as well as \( \nabla Q \), there would however be more permissible terms. Relating the constants \( L_1, L_2, L_3 \) to various integrals of \( K_{HH} \) has been done previously in [32] within the context of this model, to which we reference the reader for explicit formulae.

We now perform a similar symmetry argument here for the novel term, linear in \( \nabla Q \).

Recall from proposition 2.2 that

\[
K_{cX}(z) A \cdot B = f_1(z) \text{Tr}(AWB) + f_2(z) \text{Tr}(WA(\hat{z} \otimes \hat{z} - I)B),
\]

(119)

with \( f_1, f_2 \) isotropic functions of \( z \) and the skew-symmetric tensor \( W \) satisfying \( Wx = z \times x \).

The term in the energy linear in \( \nabla Q \) is given by

\[
VQ \cdot \nabla Q = \int_{\mathbb{R}^3} f_1(z) \text{Tr}(QW(\nabla z \cdot Q)) + f_2(z) \text{Tr}(WQ(\hat{z} \otimes \hat{z} - I)(z \cdot \nabla)Q).
\]

(120)

Integrating each part in turn we have

\[
\int_{\mathbb{R}^3} f_1(z) \text{Tr}(QW(\nabla z \cdot Q)) \, dz
\]

\[
= \int_{\mathbb{R}^3} f_1(z) Q_{ij} Q_{kl} \, dz
\]

\[
= \left( \int_{\mathbb{R}^3} f_1(z) z_\alpha z_\beta \, dz \right) \epsilon_{jmk} Q_{ij} Q_{kl}
\]

\[
= \beta_1 \epsilon_{jmk} Q_{ij} Q_{kl}
\]

(121)

The scalar \( \beta_1 \) is given by

\[
\beta_1 = \frac{1}{3} \int_{\mathbb{R}^3} f_1(z) |z|^2 \, dz = \frac{4\pi}{3} \int_0^\infty f_1(re_1) r^4 \, dr.
\]

(122)

The fact that such a scalar representation exists follows from the isotropy of \( f_1 \), which implies \( \int_{\mathbb{R}^3} z \otimes zf_1(z) \, dz \) must be a multiple of the identity.
Turning to the second term,

\[
\int_{\mathbb{R}^3} f_2(z) \text{Tr}(WQ(z \otimes \hat{z} - I)(z \cdot \nabla Q)) \, dz
\]

\[
= \int_{\mathbb{R}^3} f_2(z) W_{ij} Q_{jk} (\hat{z}_k \hat{z}_j - \delta_{kj}) z_m Q_{lm} \, dz
\]

\[
= \left( \int_{\mathbb{R}^3} f_2(z) z_n (\hat{z}_k \hat{z}_j - \delta_{kj}) z_m \, dz \right) \epsilon_{inj} Q_{jk} Q_{lm}
\]

\[
= \left( \int_{\mathbb{R}^3} f_2(z) z_n \hat{z}_k \hat{z}_j z_m - f_2(z) z_n \delta_{kj} z_m \, dz \right) \epsilon_{inj} Q_{jk} Q_{lm}.
\]

(123)

To deal with the first term in the integrand, we exploit that

\[
\frac{1}{4\pi} \int_{S^2} p_i p_j p_k p_l \, dp = \frac{1}{15} \left( \delta_{ij} \delta_{kl} + \delta_{il} \delta_{jk} + \delta_{ik} \delta_{jl} \right).
\]

This gives

\[
\int_{\mathbb{R}^3} f_2(z) z_n \hat{z}_k \hat{z}_j z_m \, dz
\]

\[
= \left( \frac{1}{4\pi} \int_{0}^{\infty} f_2(re_1) r^5 \, dr \right) \frac{1}{4\pi} \int_{S^2} p_i p_j p_k p_l \, dp
\]

\[
= \beta_2 \left( \delta_{nk} \delta_{lm} + \delta_{nl} \delta_{km} + \delta_{nm} \delta_{kl} \right).
\]

(124)

with

\[
\beta_2 = \frac{1}{15} \left( \frac{4\pi}{3} \right) \int_{0}^{\infty} f_2(re_1) r^5 \, dr.
\]

(125)

For the second term, we have by a similar argument to before,

\[
\int_{\mathbb{R}^3} f_2(z) z_n \delta_{nj} z_m \, dz = \beta_3 \delta_{nm} \delta_{kl}
\]

(126)

with

\[
\beta_3 = \frac{4\pi}{3} \int_{0}^{\infty} f_2(re_1) r^5 \, dr.
\]

(127)

Thus we return to the full expression, to give

\[
\int_{\mathbb{R}^3} f_2(z) \text{Tr}(WQ(z \otimes \hat{z} - I)(z \cdot \nabla Q)) \, dz
\]

\[
= \left( \beta_2 (\delta_{nk} \delta_{lm} + \delta_{nl} \delta_{km} + \delta_{nm} \delta_{kl}) - \beta_3 \delta_{nm} \delta_{kl} \right) \epsilon_{inj} Q_{jk} Q_{lm}
\]

\[
= \beta_2 \epsilon_{ijk} Q_{jk} Q_{li} + \beta_3 \epsilon_{ijk} Q_{jk} Q_{li} + \beta_3 \epsilon_{ijk} Q_{jk} Q_{li} - \beta_3 \epsilon_{ijk} Q_{jk} Q_{li}.
\]

(128)

Simplifying some of the terms, since \( Q_{jk} = Q_{kj} \), but \( \epsilon_{ijk} = -\epsilon_{ijk} \), this implies \( \epsilon_{ijk} Q_{jk} = 0 \).

Similarly, \( \epsilon_{inj} Q_{ni,k} = 0 \), leaving only two terms,

\[
(\beta_2 - \beta_3) \epsilon_{inj} Q_{jk} Q_{ki,n}.
\]

(129)

All in all, this gives

\[
VQ \cdot \nabla Q = (\beta_1 + \beta_2 - \beta_3) \epsilon_{ijk} Q_{jk} Q_{ki} = \beta \epsilon_{ijk} Q_{jk} Q_{ki}.
\]

(130)
\[ \beta = \frac{4\pi}{3} \int_0^\infty f_1(re_1)r^4 + \frac{1}{3}f_2(re_1)r^5 - f_2(re_1)r^4 \, dr. \quad (131) \]

5.2. Frank coefficients and HTP

Assume that \( Q \) is (at least locally) orientable, so it can be written as \( Q = s_0\sigma(n) \) for some \( n \in W^{1,2}(\Omega, S^2) \). Then the term linear in the gradient of \( Q \) becomes

\[
VQ \cdot \nabla Q = \beta \epsilon_{ijkl} Q_{ij} Q_{ik},
\]

\[
= s_0^2 \beta \epsilon_{ijkl} \left( n_i n_j - \frac{1}{3} \delta_{ij} \right) (n_i n_{k,l} + n_i n_k) \]

\[
= s_0^2 \beta \left( \epsilon_{ijkl} n_i n_{k,l} - \frac{1}{3} \epsilon_{ijkl} n_i n_k \right) \]

\[
= \beta s_0^2 n \cdot \nabla \times n. \quad (132)
\]

Combining these, and discarding an irrelevant additive constant, in the case of orientable configurations we have the \( \Gamma \)-limit as

\[
\mathcal{F}_{OF}(n) = s_0^2 \int_{\Omega} \frac{1}{2} K_{11}(\nabla \cdot n)^2 + \frac{1}{2} K_{22}(n \cdot \nabla \times n)^2 + \frac{1}{2} K_{33} |n \times \nabla \times n|^2 - \frac{s_c \beta \rho_0}{s_0} n \cdot \nabla \times n \, dx \]

\[
= s_0^2 \int_{\Omega} \frac{1}{2} K_{11}(\nabla \cdot n)^2 + \frac{1}{2} K_{22}(n \cdot \nabla \times n + q)^2 + \frac{1}{2} K_{33} |n \times \nabla \times n|^2 \, dx + C, \quad (133)
\]

where the ground state wavenumber \( q \) is given by

\[
q = - \frac{s_c \beta \rho_0}{s_0 K_{22}}, \quad (134)
\]

and the helical pitch is given by \( \frac{\pi}{q} \). Now we recall that this all takes place within a domain rescaled according to a small parameter \( \epsilon \), and that constants have been non-dimensionalised. We now rephrase (134) into our system’s original units.

\( K_{22} \) can be written as \( \frac{\mu n}{k_B T} \tilde{K}_{22} \) where \( \tilde{K}_{22} \) is a constant with units of energy depending only on the host’s structure itself, and not its temperature or concentration. Similarly, we can write \( \beta = \frac{\epsilon_{ijkl} \tilde{\beta}}{s_0} \), where \( \tilde{\beta} \) is a temperature and concentration independent quantity, depending only on the species of host and dopant. Furthermore, we recall in our scaling that lengths had been non-dimensionalised, so if the wavenumber of our system is \( q \) in dimensionless units, it is \( \tilde{q} = \frac{\pi}{q} \) in our original units. Similarly, the true concentration of dopant is \( \rho_D = \rho_0 \rho H \epsilon \). Hence reverting (134) into the original units of our problem, we have

\[
\frac{1}{\tilde{q}} = - \frac{s_c \mu n}{\rho H s_0 \frac{\mu n}{k_B T} \tilde{K}_{22}} \tilde{\beta} \rho_D \\
\Rightarrow \tilde{q} = - \frac{s_c \tilde{\beta} \rho_D}{\rho H s_0 \tilde{K}_{22}}. \quad (135)
\]

Thus this gives our expression for the helical twisting power in dilute systems, as
Again, we emphasise that $\tilde{\beta}, K_{22}$ are temperature and concentration independent, defined entirely in terms of the pairwise host–dopant and host–host interactions, respectively. The temperature dependence of $h$ is thus encoded entirely within the ratio of the order parameters $s_c, s_0$, and generally we expect this to be a highly nonlinear description. However as $s_0, s_c$ solve one-dimensional minimisation problems, it is an elementary exercise to numerically illustrate the temperature dependence.

The value of $s_0$ is determined entirely by $k_{HH}^0$, which can be written as $k_{HH}^0 = \frac{\rho h k_B}{k_1 T}$ for a temperature and concentration independent constant $k_1$. There are explicit formulae for the relationship between $s_0$ and $k_{HH}^0$, available in [9]. The order parameter $s_c$ is determined entirely by $k_{HD}^0 = \frac{\rho h k_B}{k_2 T}$, where again $k_2$ is temperature and concentration dependent. $s_c$ can be explicitly obtained from $s_0$ as

$$s_c = \frac{\int_{-1}^1 P_2(x) \exp\left(\frac{k_{HD}^0 s_0 P_2(x)}{\rho h k_B}ight) dx}{\int_{-1}^1 \exp\left(\frac{k_{HD}^0 s_0 P_2(x)}{\rho h k_B}ight) dx},$$

(137)

where $P_2(x) = \frac{1}{2} (3x^2 - 1)$ is the second Legendre polynomial, satisfying $\sigma(p) \cdot \sigma(q) = \frac{2}{3} P_2 (p \cdot q)$ which follows from (82) and (24). We define a rescaled temperature $\tau = \frac{k_B T}{\rho h}$, and parameter $\alpha = \frac{k_2}{k_1} = \frac{K_{HD}}{k_B}$, which satisfies $\frac{\rho h}{k_B} T \tau = \rho h \frac{k_B}{k_1}$. From these we present the dependence of $h$, or more appropriately the dimensionless quantity $\hat{h} = \frac{k_{HD}^0 s_0}{\rho h k_B} h = \frac{h}{\hat{h}}$, in terms of $\tau$ for representative values of $\alpha$. We define $\hat{h}$ as it is the only contribution to the HTP that is explicitly temperature dependent.

Notably, when $\alpha = 1$, $h$ is independent of the temperature. To see this, first we define the scalar function $\lambda : (-\frac{1}{2}, 1) \to \mathbb{R}$, related to $\Lambda : \mathcal{Q} \to \text{Sym}_0(3)$ as in proposition 2.4, by

$$\lambda(s) = \frac{3}{2} \Lambda(s \sigma(n)) \cdot \sigma(n),$$

(138)

where by frame invariance the choice of $n \in S^2$ does not affect the definition. Using this notation, the dependence of $s_0, s_c$ on material constants and parameters can be seen through their critical point conditions. Noting the full tensorial critical point conditions for $\xi, Q$ are

$$0 = \Lambda(Q) - \frac{1}{\tau} Q, \quad 0 = \Lambda(\xi) - \frac{\alpha}{\tau} Q,$$

(139)

we recall $Q = s_0 \sigma(n), \xi = s_c \sigma(n)$ for some $n \in S^2$, so by taking the inner product of the equation (139) against $\sigma(n)$ we obtain the scalar critical point conditions for $s_0, s_c$ as

$$0 = \lambda(s_0) - s_0, \quad 0 = \lambda(s_c) - s_0 \tau,$$

(140)

Thus when $\alpha = 1, \lambda(s_c) = \lambda(s_0)$ so $s_c = s_0$ and $\hat{h} = 1$. Recalling the definition of $\alpha$, $\alpha = 1$ corresponds to the case where $k_{HH}^0 = k_{BD}^0$. That is, the (average) host–host interaction is equal to that of the host–dopant interaction.
Furthermore, we can write
\[ \tilde{h} = \frac{s_c}{s_0} = \frac{\lambda^{-1} \left( \frac{\alpha s_0}{\tau} \right)}{\lambda^{-1} \left( \frac{s_0}{\tau} \right)}. \]  
\[ (141) \]
As \( \lambda^{-1} \) is strictly increasing, this implies that if \( \alpha < 1 \), \( \tilde{h} < 1 \), and if \( \alpha > 1 \), \( \tilde{h} > 1 \). We also see that as \( \tau \to 0 \), as \( s_c, s_0 \to 1 \), this means \( \tilde{h} \to 1 \). We also see that as \( \alpha \to 0 \), \( \tilde{h} \) must be approximately linear in \( \alpha \), and as \( \alpha \to \infty \), \( s_c \to 1 \) so \( \tilde{h} \to \frac{1}{s_0} \). We show the numerically found results in figure 1, for \( \alpha = 0.15 \) showing a decreasing, convex dependence on \( \tau \), \( \alpha = 0.75 \) showing a concave, decreasing dependence on \( \tau \), and \( \alpha = 2 \), showing a convex increasing dependence on \( \tau \).

We also include a contour plot in figure 2 showing a range of \( (\tau, \alpha) \) space and the corresponding values of \( \tilde{h} \).

Figure 1. Plots of \( \tilde{h} \) as a function of \( \tau \), for representative values of \( \alpha \). (a) \( \alpha = 0.15 \). (b) \( \alpha = 0.75 \). (c) \( \alpha = 2 \).

Figure 2. A contour plot of the dimensionless HTP \( \tilde{h} \) plotted against parameters \( \alpha, \tau \).
6. Conclusions

Within this work we have proposed a mean-field model for a spatially inhomogeneous two-species host–dopant mixture based on simple pairwise interactions. The type of pairwise interactions considered are based on leading order contributions to dispersion forces at large molecular separation, which tend to dominate in larger, apolar molecules. Both formally and in the language of Γ-convergence, we have analysed the asymptotics of this model in a large-domain and dilute-dopant limit, where the dopant number density scales as the reciprocal of domain size. This gives the Oseen–Frank free energy for cholesterics, where the Frank constants and ground state wavenumber admit explicit representations in terms of the molecular interactions and equilibrium order parameters of the two species. Due to the nature of the scaling, the formulation is valid in only large-wavelength regimes, with emergent behaviour in highly-doped and and short-wavelength cholesterics remaining avenues for future investigation. In particular, this work gives an expression for the HTP, which may be increasing, decreasing or independent with respect to temperature depending on the relative strength of the host–host and host–dopant interactions, qualitatively respecting the experimental fact that a different dopant may have positive or negative temperature dependence with the same host system. Unfortunately as detailed information of the molecular interactions is required to obtain the relevant material parameters, this makes quantitative comparison with experiment difficult.

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\[ S^2 \] The unit sphere in \( \mathbb{R}^3 \).

\[ \mathcal{P}(S^2) \] The set of \( L^1 \) probability distributions on \( S^2 \).

\[ \text{Sym}_3(\mathbb{R}) \] The set of traceless symmetric \( 3 \times 3 \) matrices.

\( \epsilon_{ijk} \) Levi-Civita symbol.

\( k_B \) Boltzmann constant.

\( X \cdot Y \) The Euclidean inner product of two tensors of equal rank \( X, Y \).

\( \otimes \) The tensor product.

\( |X| \) The Euclidean norm of a vector \( X \) or the Frobenius norm of a matrix \( X \).

\( \lambda_{\text{min}}(A)/\lambda_{\text{max}}(A) \) The smallest/largest (respectively) eigenvalue of a matrix \( A \).

\( Q \) The subset of \( \text{Sym}_3(\mathbb{R}) \) containing matrices \( Q \) with \( \lambda_{\text{min}}(Q) > -\frac{1}{3} \).

\( \psi_\gamma \) The convex part of the singular Ball–Majumdar potential.

\( K_{XX} \) The tensor describing the chiral contribution to the interaction between species \( X \) and the chiral dopant.

\( K_{XY} \) The tensor describing the achiral contribution to the interaction between species \( X \) and \( Y \).

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Appendix A

A.1. Notation

A.2. Proof of proposition 2.1

Proof. The condition (11) immediately implies that
\[
R \left( \tilde{K}_{XY}^a(z) \sigma(p) \right) R^T = \tilde{K}_{XY}^a(Rz) \sigma(Rp) \tag{A.1}
\]
for all \( R \in \text{SO}(3), z \in \mathbb{R}^3, p \in S^2 \). Given any traceless, symmetric matrix \( A \), by eigenvalue decomposition it may be written as \( A = \sigma(e_1) + r \sigma(e_2) \), where \( e_1, e_2 \) are unit eigenvectors with corresponding eigenvalues \( \frac{\sigma - \epsilon}{2} \), \( \frac{\sigma + \epsilon}{2} \), respectively. Thus, since \( \sigma(Rp) = R \sigma(p) R^T \) and (A.1) is linear in \( \sigma(p) \), we have
\[
R \left( \tilde{K}_{XY}^a(z) A \right) R^T = \tilde{K}_{XY}^a(Rz)(RAR^T) \tag{A.2}
\]
for all \( z \in \mathbb{R}^3, A \in \text{Sym}_0(3) \) and \( R \in \text{SO}(3) \). As this therefore defines a frame invariant function from \( \mathbb{R}^3 \times \text{Sym}_0(3) \ni (z,A) \mapsto \tilde{K}_{XY}^a(z) A \in \text{Sym}_0(3) \), by [30] we may write
\[
\tilde{K}_{XY}^a(z) A = \tilde{k}_1(z,A) A + \tilde{k}_2(z,A) (Az \otimes z + z \otimes Az) + \tilde{k}_3(z,A)(Az \cdot z)z \\
\otimes z + \tilde{k}_4(z,A) Az \otimes Az + \tilde{k}_5(z,A) A^2 + \tilde{k}_6(z,A) I, \tag{A.3}
\]
where the scalar valued functions \( \tilde{k}_i(z,A) \) satisfy
\[
\tilde{k}_i(z,A) = \kappa_i(|z|, \text{Tr}(A), \text{Tr}(A^2), \text{Tr}(A^3), z \cdot Az, z \cdot A^2 z). \tag{A.4}
\]
However, as the map is linear in \( A \), we see that we may disregard all terms nonlinear in \( A \), in which case it reduces to
\[
\tilde{K}_{XY}^a(z) A = k_1(z) A + k_2(z) (Az \otimes z + z \otimes Az) + k_3(z)(Az \cdot z)z \otimes z + \tilde{k}_6(z,A) I, \tag{A.5}
\]
with \( k_i \) depending only on \( |z| \) for \( i = 1, 2, 3 \). Finally, as \( \tilde{K}_{XY}^a(z) A \) is required to be traceless, and \( A \) itself is traceless, by setting the trace of (A.5) to zero, we establish that the only choice for \( \tilde{k}_6(z,A) \) is given by
\[
\tilde{k}_6(z,A) = -\frac{Az \cdot z}{3} \left( 2k_2(z) + k_3(z)|z|^2 \right). \tag{A.6}
\]
□

A.3. Proof of proposition 2.2

Proof. As
\[
\tilde{K}_{ix}(z) \sigma(p) \cdot \sigma(q) = \tilde{K}_{ix}(Rz) \sigma(Rp) \cdot \sigma(Rq), \\
\tilde{K}_{ix}(-z) = -\tilde{K}_{ix}(z), \\
\sigma(-p) = \sigma(p), \tag{A.7}
\]
for all \( p, q \in S^2, z \in \mathbb{R}^3, R \in \text{O}(3) \), we have
\[
\tilde{K}_\mathcal{X}(Rz)\sigma(Rp) = \text{Det}(R)R\left(\tilde{K}_\mathcal{X}(z)\sigma(p)\right)R^T
\]  
(A.8)

for all \( z \in \mathbb{R}^3, p \in S^2, R \in O(3) \). Similarly to the proof of proposition 2.1, this implies that for all \( A \in \text{Sym}_0(3) \),
\[
\tilde{K}_\mathcal{X}(Rz)(RAR^T) = \text{Det}(R)R\left(\tilde{K}_\mathcal{X}(z)A\right)R^T.
\]  
(A.9)

That is to say, that the map \((z, A) \mapsto \tilde{K}_\mathcal{X}(z)A\) is hemitropic, a function invariant under proper rotations, but admits a sign change under improper rotations. Using the expressions given in [section 4.4] for such hemitropic functions, by a similar argument to proposition 2.1 we may thus write, by keeping only the linear terms, that
\[
\tilde{K}_\mathcal{X}(z)A = f_1(z)(AW - WA) + f_2(z)(WAW^2 - W^2AW) + f_3(z)A + f_4(z)WAW + f_5(z, A)z \otimes z.
\]  
(A.10)

Here the skew-symmetric matrix \( W \) is defined by \( Wx = z \times x \), and the functions \( f_i \) must be frame invariant. We now show that \( f_1, f_2, f_3 \) must be zero. As \( \tilde{K}_\mathcal{X}(z)A \) must have odd-symmetry in \( z \), we conclude that \( f_1, f_2, f_3 \) must also have odd symmetry in \( z \). As \( f_3, f_4 \) depend only on \(|z|\), this must mean that they are identically zero. Turning to \( f_5 \), we can write that
\[
f_5(z, A) = \tilde{f}_5(|z|, \text{tr}^2, \text{tr}A^2, z \cdot A, z \cdot A^2, z \cdot A \times A^2, z, z). \]  
(A.11)

However, as \( f_5 \) is required to be linear in \( A \) and have odd symmetry in \( z \), this must be of the form \( g_5(z)z \cdot A \) for odd, isotropic \( g_5 \), therefore \( g_5 \) must be zero also and \( f_5 = 0 \).

We can furthermore simplify the expression by noting the identity that
\[
W^2x = z \times (z \times x) = (z \cdot x)z - (z \cdot z)x = |z|^2 (\tilde{z} \otimes \tilde{z} - I)x,
\]  
(A.12)

so that \( W^2 = |z|^2 (\tilde{z} \otimes \tilde{z} - I) \). Furthermore, we will make use of more explicit expressions when the traceless symmetric matrices are uniaxial. It is then a tedious but straightforward exercise to verify that for \( \sigma_1 = \sigma(p), \sigma_2 = \sigma(q) \),
\[
\text{Tr}(\sigma_1 W \sigma_2) = (z \cdot p \times q)(p \cdot q),
\]
\[
\text{Tr}(W \sigma_1 W^2 \sigma_2) = (z \cdot p \times q)(p \cdot z)(q \cdot z) - |z|^2 (z \cdot p \times q)(p \cdot q).
\]  
(A.13)

At other points it may be more useful to consider a full tensorial form. If \( Q^1, Q^2 \) are symmetric, traceless tensors, then we can write
\[
\text{Tr}(Q^1 W Q^2) = Q^1_{ij} \epsilon_{ijkz} Q^2_{jk},
\]
\[
\text{Tr}(W Q^1 W^2 Q^2) = |z|^2 \epsilon_{ijkz} Q^1_{kl}(\tilde{z} \tilde{z} m - \delta_{lm}) Q^2_{mj}.
\]  
(A.14)

### A.4. Proof of proposition 2.5

Before moving on to the proof of proposition 2.5, we include a necessary lemma.

**Lemma A.1.** Let \( Q_1, Q \in L^{\infty}(\Omega, \mathbb{Q}) \). Assume that \( Q_1 \rightarrow Q \) pointwise almost everywhere, \( \int_{\Omega} \psi_\epsilon(Q_1(x)) \, dx \) is bounded and \( \int_{\Omega} \psi_\epsilon(Q(x)) \, dx \) is finite. Then \( f_{Q_1} \rightarrow f_Q \) in \( L^1 \).

**Proof.** As \( \int_{\Omega} \psi_\epsilon(Q_1(x)) \, dx = \int_{\Omega \times \mathbb{R}^3} f_{Q_1}^{\infty}(x, p) \ln f_{Q_1}^{\infty}(x, p) \, d(x, p) \) is bounded, we have that \( f_{Q_1}^{\infty} \) is a uniformly integrable sequence. Furthermore, by the assumptions of the lemma we have that for every \( \epsilon > 0 \), there exists some \( \gamma > 0 \) and \( U_\epsilon \subset \Omega \) so that
- \( d(Q(x), \partial Q) > \gamma \) for almost every \( x \in U_\epsilon \).

- \( Q^j \to Q \) uniformly on \( U_\epsilon \).

- \( |\Omega \setminus U_\epsilon| < \epsilon \).

To show such a \( U_\epsilon \) exists, first we take \( U_\epsilon^j \) to be so that \( Q^j \to Q \) uniformly on \( U_\epsilon^j \), with \( |\Omega \setminus U_\epsilon^j| < \frac{\epsilon}{2} \), which is permissible by Egorov’s theorem. Then take \( \gamma \) sufficiently small so that \( U_\epsilon = \{ x \in U_\epsilon^j : \gamma(x) = \partial Q \to \gamma \} \) satisfies the final equality. Furthermore, for \( j \) sufficiently large, we have that \( d(Q^j(x), \partial Q) > \gamma \) almost everywhere in \( U_\epsilon \).

As \( \Lambda \) is a smooth function of its argument, and \( f^Q \) depends on \( \Lambda(Q) \) smoothly, this implies that \( Q \to f^Q \) is Lipschitz from \( \text{Sym}_1(\Omega) \) to \( L^1 \) on compact subsets of \( \Omega \). This means that we may estimate, for \( j \) sufficiently large,

\[
\int_{\Omega \times \mathbb{S}^2} |f^j(x,p) - f(x,p)| \, d(x,p) = \int_{U_\epsilon \times \mathbb{S}^2} |f^j(x,p) - f(x,p)| \, d(x,p) + \int_{U_\epsilon^j \times \mathbb{S}^2} |f^j(x,p) - f(x,p)| \, d(x,p) \\
\leq C \int_{U_\epsilon} |Q^j(x) - Q(x)| \, dx + \int_{U_\epsilon^j \times \mathbb{S}^2} |f^j(x,p) - f(x,p)| \, d(x,p) \\
\Rightarrow \limsup_{j \to \infty} \int_{\Omega \times \mathbb{S}^2} |f^j(x,p) - f(x,p)| \, d(x,p) \leq \limsup_{j \to \infty} \int_{U_\epsilon^j \times \mathbb{S}^2} |f^j(x,p) - f(x,p)| \, d(x,p). \tag{A.15}
\]

Here, \( C \) denotes the Lipschitz constant of \( Q \to f^Q \) on the set of \( Q \) with \( d(Q, \partial Q) > \gamma \).

We note that for the right-hand limit superior, this is a bounded quantity in \( j \) as \( f^j \) is uniformly integrable and \( f \) is integrable, and further more may be made arbitrarily small by taking \( \epsilon \) sufficiently small. This then implies that

\[
\limsup_{j \to \infty} \int_{\Omega \times \mathbb{S}^2} |f^j(x,p) - f(x,p)| \, d(x,p) = 0. \tag{A.16}
\]

Hence we have \( L^1 \) convergence.

Now we move on to the proof of proposition 2.5

**Proof.** For notational simplicity, let \( \mathcal{H} \) denote the entropy,

\[
\mathcal{H}(f) = k_B T \int_{\mathbb{S}^2} f(x,p) \ln f(x,p) \, d(x,p). \tag{A.17}
\]

Let \( Q[f] \) denote the Q-tensor of \( f \),

\[
Q[f](x) = \int_{\mathbb{S}^2} f(x,p) \sigma(p) \, dp. \tag{A.18}
\]

and let \( B(Q, \xi) \) denote the bilinear form

\[
B(Q, \xi) = -\frac{\rho_\Omega}{2} \int_{\Omega} \int \tilde{K}_{DD}(x-y) \xi(x) \cdot \xi(y) + \tilde{K}_{D}(x-y) \xi(x) \cdot \xi(y) \, dx \, dy \\
- \frac{\rho_\Omega}{2} \int_{\Omega} \int \tilde{K}_{HH}(x-y) Q(x) \cdot Q(y) \, dx \, dy \\
- \rho_{D\Omega} \int_{\Omega} \int (\tilde{K}_{HD}(x-y) Q(x) \cdot \xi(y) + \tilde{K}_{DH}(x-y) Q(x) \cdot \xi(y)) \, dx \, dy. \tag{A.19}
\]
Then $G$ can be expressed as
\[ G(f_H, f_D) = p_H \mathcal{H}(f_H) + p_D \mathcal{H}(f_D) + B(Q[f_H], Q[f_D]). \]  
(A.20)

First we note that by Fubini, for almost every $x \in \Omega$ and $X = H, D$, $f_X(x, \cdot) \in \mathcal{P}(\mathbb{S}^2)$. Take $f_X$ to have finite entropy, which implies we may define $\int_{\mathbb{S}^2} f(x, p) \ln f(x, p) \, dp$ for almost every $x$. Employing Fubini again, we note that
\begin{align*}
\int_{\Omega \times \mathbb{S}^2} f_X(x, p) \ln f_X(x, p) \, d(x, p) &= \int_{\Omega} \left( \int_{\mathbb{S}^2} f_X(x, p) \ln f_X(x, p) \, dp - \psi_s(Q[f_X](x)) \right) \, dx \\
&= \int_{\Omega} \left( \int_{\mathbb{S}^2} f_X(x, p) \ln f_X(x, p) \, dp - \psi_s(Q[f_X](x)) \right) \, dx.
\end{align*}
(A.21)

By the definition of $\psi_s$, we have that the inner integral is non-negative for almost every $x$, and zero if and only if for almost every $x \in \Omega$, $f_X(x, p) = f^{Q[f_X]}(x)(p)$ for almost every $p \in \mathbb{S}^2$. That is to say, that $\mathcal{H}(f) \geq \mathcal{H}(f^{Q[f_X]}(x))$, with equality if and only if $f(x, p) = f^{Q[f_X]}(x)(p)$ for almost every $(x, p)$.

Suppose that $f_H, f_D$ are an $L^1$-local minimising pair for the energy $G$, with corresponding Q-tensors $Q[f_H], Q[f_D]$, and there exists a positive measure set so that $X$ equal to $H$ or $D$, $f_X(x, p) \neq f^{Q[f_X]}(x)(p)$, by strict convexity of entropy we have that for $f_X^\delta = (1 - \delta) f_X + \delta f^{Q[f_X]}$, $1 > \delta > 0$
\[ \mathcal{H}(f_X^\delta) < (1 - \delta) \mathcal{H}(f_X) + \delta \mathcal{H}(f^{Q[f_X]}) < \mathcal{H}(f_X) \]  
(A.22)
as $Q[f_X^\delta] = Q[f_X]$, this implies that
\begin{align*}
G(f_H, f_D) &= p_H \mathcal{H}(f_H) + p_D \mathcal{H}(f_D) + B(Q[f_H], Q[f_D]) \\
&= p_H \mathcal{H}(f_H) + p_D \mathcal{H}(f_D) + B(Q[f_H^\delta], Q[f_D^\delta]) \\
&> p_H \mathcal{H}(f_H^\delta) + p_D \mathcal{H}(f_D^\delta) + B(Q[f_H^\delta], Q[f_D^\delta]) \\
&= G(f_H^\delta, f_D^\delta).
\end{align*}
(A.23)

Furthermore, as $f_X^\delta \to f_X$ strongly in $L^1$ as $\delta \to 0$, we can not have that $f_H, f_D$ is a local $L^1$-minimising pair, as $f_H^\delta, f_D^\delta$ are competitors with lower energy. This implies that all $L^1$-local minimisers are of the form $f_H = f^O, f_D = f^S$ where $Q, \xi$ are their corresponding Q-tensors. Now we show that an $L^1$-local minimiser of $G$, of this form, corresponds to an $L^1$-local minimising pair $(Q, \xi)$ of $F$. Let $(Q^\delta, \xi^\delta) \to (Q, \xi)$ in $L^1$. Let us presume that $\liminf_{\delta \to 0} p_H \Psi_s(Q^\delta) + p_D \Psi_s(\xi^\delta) < +\infty$, else $(Q^\delta, \xi^\delta)$ cannot be a successful energetic competitor. Then we take a subsequence $Q^\delta = Q^\delta, \xi^\delta = \xi^\delta$ so that the energy converges to the limit inferior, we must have that $f^O, f^S$ have bounded entropy. By lemma A.1, we have that $(f^O, f^S) \to (f^O, f^S)$ strongly in $L^1$. Therefore, as $(f^O, f^S)$ is an $L^1$-local minimising pair,
\begin{align*}
F(Q, \xi) &= G(f^O, f^S) \\
&\leq G(f^O, f^S) \\
&= F(Q, \xi).
\end{align*}
(A.24)

Now we presume that $Q, \xi$ are an $L^1$-minimising pair for $F$. For notational simplicity, define $\Psi_s$ by
\[
\Psi_s(Q) = \int_{\Omega} \psi_s(Q(x)) \, dx. \tag{A.25}
\]

Now presume that \( f_H^\delta, f_D^\delta \) are such that \( f_H^\delta \to f_H \) strongly in \( L^1 \), where \( f_H = fQ, f_D = f\xi \). We note that \( f \mapsto Q[f] \) is continuous from \( L^1 \) to \( L^1 \), so that \( Q[f_H^\delta] \to Q[f_H] \) as \( \delta \to 0 \) in \( L^1 \). Therefore we have that for \( \delta \) sufficiently small,
\[
\mathcal{G}(f_H, f_D) = \rho_H \Psi_s(Q) + \rho_D \Psi_s(\xi) + B(Q, \xi) \\
\leq \rho_H \Psi_s(Q[f_H^\delta]) + \rho_D \Psi_s(Q[f_D^\delta]) + B(Q[f_H^\delta], Q[f_D^\delta]) \\
\leq \rho_H \mathcal{H}(f_H^\delta) + \rho_D \mathcal{H}(f_D^\delta) + B(Q[f_H^\delta], Q[f_D^\delta]) \\
= \mathcal{G}(f_H^\delta, f_D^\delta). \tag{A.26}
\]

Therefore \( f_H, f_D \) is an \( L^1 \)-local minimising pair for \( \mathcal{G} \). □

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