Numerical calculations of the phase diagram of cubic blue phases in cholesteric liquid crystals

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Abstract

We study the static properties of cubic blue phases by numerically minimising the three-dimensional, Landau-de Gennes free energy for a cholesteric liquid crystal close to the isotropic-cholesteric phase transition. Thus we are able to refine the powerful but approximate, semi-analytic frameworks that have been used previously. We obtain the equilibrium phase diagram and discuss it in relation to previous results. We find that the value of the chirality above which blue phases appear is shifted by 20% (towards experimentally more accessible regions) with respect to previous estimates. We also find that the region of stability of the $O_5$ structure – which has not been observed experimentally – shrinks, while that of BP I ($O_8^-$) increases thus giving the correct order of appearance of blue phases at small chirality. We also study the approach to equilibrium starting from the infinite chirality solutions and we find that in some cases the disclination network has to assemble during the equilibration. In these situations disclinations are formed via the merging of isolated aligned defects.

61.30.Mp,83.80.Xz,61.30.Dk
I. INTRODUCTION

Liquid crystals are typically composed of highly anisotropic molecules. They are viscoelastic materials; some of their properties are typical of a liquid while others are usually associated with solids. As liquids, they can flow and they exhibit a viscous response to an applied stress. However, liquid crystals also possess long-range, orientational order [1,2] which results from the entropic advantage of aligning the constituent molecules. The long-range, orientational order is usefully described by the director field $\vec{n}$, the coarse-grained, average, molecular orientation. In a cholesteric or chiral nematic liquid crystal $\vec{n}$ has a natural twist deformation along an axis perpendicular to the molecules [1,2]. Examples of cholesteric liquid crystals are DNA molecules in solution, colloidal suspensions of bacteriophages [3], and solutions of nematic mixtures such as E7 with chiral dopants which are widely used in display devices.

A particularly intriguing phase of liquid crystals is obtained by slowly cooling down a liquid crystal from the isotropic into the cholesteric phase. Instead of a direct transition into a helical configuration, it was found experimentally that the system passes through a series of first order phase transitions, all of which occur in a temperature range of roughly 1K [4,5]. These phases are known as blue phases. Typically [4], experiments report a series of at least three phases intervening in this small temperature range. The series of transitions is often as follows: isotropic (I) $\rightarrow$ blue phase III (BP III) $\rightarrow$ blue phase II (BP II) $\rightarrow$ blue phase I (BP I) $\rightarrow$ cholesteric (C). BP I and BP II display a cubic symmetry, while BP III has an amorphous nature. Blue phases are now beginning to find applications in lasers [6] and in electric field driven devices [7].

Blue phases provide a particularly fascinating example of liquid crystal ordering as they correspond to complicated director fields which, even in equilibrium, are threaded by a regular network of disclinations [8–13]. Identifying their structure presented a considerable theoretical challenge the resolution of which is clearly summarised in the review by Wright and Mermin [4].
In the literature attention has mainly focussed on four different candidates for the cubic blue phases. The nomenclature used here refers to the symmetry group which characterises the lattice of disclinations formed in the blue phases following [4,11,12]. O\textsubscript{2} has the symmetry of a simple cubic lattice, O\textsubscript{8}\textsuperscript{+}\textsuperscript{−} and O\textsubscript{5} that of a body-centered-cubic lattice. The two O\textsubscript{8} phases are candidates for BP I as they have the same octahedral symmetry, while O\textsubscript{2} has been proposed as a model for BP II. The defect structure in each phase in shown in Figure 1. In O\textsubscript{2} and in O\textsubscript{5} the defect lines merge in the center of the unit cell, whereas in the octahedral phases the defects avoid each other.

The Q tensor theory, in which the local conformation of the liquid crystal is specified by a tensor, and not only by the director field \( \vec{n} \), is the natural language to understand the equilibrium properties of blue phases because it is able to capture their inherent biaxiality \[4\]. With the advent of more powerful computers it is now possible to numerically minimise the free energy for any value of the chirality \( \kappa \) without further approximation than that inherent in the free energy expression itself. This is the programme we follow in this paper.

We determine the equilibrium phase diagram which specifies which of the cubic blue phases has the lowest free energy as a function of the system parameters. We find a phase diagram qualitatively similar to that found in earlier work and compatible with the assignments BP I = O\textsubscript{8}\textsuperscript{−} and BP II = O\textsubscript{2}. However there are quantitative differences. In particular the results show that the triple point between the cholesteric and blue phases is lowered in chirality by around 20\%. We also show that the region of stability of O\textsubscript{5} shrinks and that of O\textsubscript{8}\textsuperscript{−} increases with respect to the previous estimates. The revised phase diagram is more compatible with observations suggesting that the Landau-de Gennes theory is sufficient to explain the static observations on blue phases. Finally, we characterise the approach to equilibrium and in particular we describe the dynamic pathway by which the disclination structure of O\textsubscript{8}\textsuperscript{−} assembles in the simulations.
II. LANDAU-DE GENNES THEORY FOR CHOLESTERIC BLUE PHASES

The equilibrium properties of the liquid crystal are described by a Landau-de Gennes free energy density expanded in terms of a tensor order parameter $Q$. This is related to the direction of individual molecules, $\hat{n}$, by $Q_{\alpha\beta} = \langle \hat{n}_\alpha \hat{n}_\beta - \frac{1}{3} \delta_{\alpha\beta} \rangle$ where the angular brackets denote a coarse-grained average and the Greek indices label the Cartesian components of $Q$. The tensor $Q$ is traceless and symmetric. Its largest eigenvalue, $\frac{2}{3}q$, $0 < q < 1$, describes the magnitude of the order.

The free energy comprises a bulk term $F_b$ (summation over repeated indices is implied hereafter in our notation)

$$F_b = \frac{A_0}{2} \left( 1 - \frac{\gamma}{3} \right) Q_{\alpha\beta}^2 - \frac{A_0 \gamma}{3} Q_{\alpha\beta} Q_{\beta\gamma} Q_{\gamma\alpha} + \frac{A_0 \gamma}{4} (Q_{\alpha\beta}^2)^2$$

and a distortion term, $F_d$ which for cholesterics is [1,4]

$$F_d = \frac{K}{2} \left[ (\partial_{\beta} Q_{\alpha\beta})^2 + (\epsilon_{\alpha\zeta\delta} \partial_{\zeta} Q_{\delta\beta} + 2q_0 Q_{\alpha\beta})^2 \right]$$

where $K$ is an elastic constant and $q_0 = 2\pi/p$, with $p$ the pitch of the cholesteric liquid crystal. The tensor $\epsilon_{\alpha\zeta\delta}$ is the Levi-Civita antisymmetric third-rank tensor, $A_0$ is a constant and $\gamma$ controls the magnitude of the order (physically it corresponds to an effective temperature or concentration for thermotropic and lyotropic liquid crystal respectively). This free energy has the same functional form of the one employed in Refs. [9,10], but the latter is more general as it contains one more parameter in the bulk free energy density term.

Of particular interest for the present discussion of blue phase equilibrium [4] are two quantities, the chirality $\kappa$, and the reduced temperature $\tau$. These are defined in Ref. [10] and in our formulation they can be found via:

$$\kappa = \sqrt{\frac{108Kq_0^2}{A_0 \gamma}}$$

$$\tau = \frac{27A_0 (1 - \gamma/3) + 108Kq_0^2}{A_0 \gamma} = \frac{27(1 - \gamma/3)}{\gamma} + \kappa^2.$$

Approaches to study the equilibrium properties of blue phases which have given a great deal of insight into the phase behaviour have so far been based on an expansion in the
parameter $\kappa$. *High chirality* theories are strictly valid for infinite $\kappa$. In that case an infinite number of exact minimizers of the free energy density can be found as an arbitrary sum of biaxial helices [4]. *Low chirality* theories have also been formulated. These rely on the Frank free energy defined in terms of the coarse grained director field $\vec{n}$ instead of $\mathbf{Q}$; this is equivalent to assuming a uniaxial order parameter.

In this work we do not make assumptions about the value of $\kappa$ but rather minimise the Landau-de Gennes free energy by numerically solving an equation of motion for $\mathbf{Q}$ [14]

$$\frac{\partial Q_{\alpha\beta}}{\partial t} = \Gamma H_{\alpha\beta} \tag{4}$$

where $\Gamma$ is a collective rotational diffusion constant.

The term on the right-hand side of Eq. (4) describes the relaxation of the order parameter towards the minimum of the free energy. The molecular field $\mathbf{H}$ which provides the driving force is related to the derivative of the free energy $F$ by

$$\mathbf{H} = -\frac{\delta F}{\delta \mathbf{Q}} + \left(\frac{1}{3}\right) Tr \frac{\delta F}{\delta \mathbf{Q}} \tag{5}$$

where $Tr$ denotes the tensorial trace. From Eqs. (1) and (2), the molecular field is explicitly

$$H_{\alpha\beta} = \left( A_0 (1 - \gamma/3) + 4Kq_0^2 \right) Q_{\alpha\beta} - A_0 \gamma \left( Q_{\alpha\gamma} Q_{\gamma\beta} - \frac{\delta_{\alpha\beta}}{3} Q_{\gamma\delta}^2 \right) + A_0 \gamma Q_{\gamma\delta}^2 Q_{\alpha\beta} + K \partial_{\gamma}^2 Q_{\alpha\beta} - 4Kq_0 \epsilon_{\alpha\gamma\delta} \partial_{\gamma} Q_{\delta\beta}. \tag{6}$$

**III. NUMERICAL ALGORITHM**

Our aim in this work is to numerically minimise – by solving Eq. (4) using a lattice Boltzmann algorithm – the free energies of the cubic blue phases $O_2$, $O_5$, $O_8^+$ and $O_8^-$. In this Section we report the procedure used.

The equilibrium state for chosen values of chirality $\kappa$ and reduced temperature $\tau$ was obtained as the steady state solution of the equation of motion (4). The initial condition for each phase was taken as its configuration for infinite chirality ($\kappa = \infty$ or $A_0 = 0$) for which
exact analytical expressions are available [4]. In the $\kappa = \infty$ limit the $Q$ tensors characterising the blue phases retain the correct topology of the disclination lines. As expected this was preserved under the dynamics allowing us to minimise the free energy for a structure with the chosen network of disclinations for any value of $\tau$ and $\kappa$.

For completeness we report here the initial configurations chosen in this work. (Note that in all cases the components $yy$, $zz$, $xz$ and $yz$ are obtained by cyclic permutation from those given below.)

The initial configuration for $O_2$ is

$$Q_{xx} = A \{\cos (2q_0 z) - \cos (2q_0 y)\}, \quad Q_{xy} = -A \sin (2q_0 z)$$

where $A > 0$ is an arbitrary amplitude.

That for $O_5$ is

$$Q_{xx} = A \{2 \cos (\sqrt{2}q_0 y) \cos (\sqrt{2}q_0 z)$$

$$- \cos (\sqrt{2}q_0 x) \cos (\sqrt{2}q_0 z) - \cos (\sqrt{2}q_0 x) \cos (\sqrt{2}q_0 y)\},$$

$$Q_{xy} = A \{\sqrt{2} \cos (\sqrt{2}q_0 y) \sin (\sqrt{2}q_0 z)$$

$$- \sqrt{2} \cos (\sqrt{2}q_0 x) \sin (\sqrt{2}q_0 z) - \sin (\sqrt{2}q_0 x) \sin (\sqrt{2}q_0 y)\}$$

where $A > 0$.

Those for $O_8^{+,-}$ are

$$Q_{xx} = A \{-2 \cos (\sqrt{2}q_0 y) \sin (\sqrt{2}q_0 z)$$

$$+ \sin (\sqrt{2}q_0 x) \cos (\sqrt{2}q_0 z) + \cos (\sqrt{2}q_0 x) \sin (\sqrt{2}q_0 y)\}$$

$$Q_{xy} = A \{\sqrt{2} \cos (\sqrt{2}q_0 y) \cos (\sqrt{2}q_0 z)$$

$$+ \sqrt{2} \sin (\sqrt{2}q_0 x) \sin (\sqrt{2}q_0 z) - \sin (\sqrt{2}q_0 x) \cos (\sqrt{2}q_0 y)\}$$

where $A$ is positive for $O_8^+$ and negative for $O_8^-$. 6
In general, the minimum free energy for blue phases is not attained when the periodicity of the disclination lattice matches the pitch of the cholesteric helix $p$ but when the unit cell is larger. This is accounted for by considering alternative initial conditions with $q_0$ substituted by $rq_0$ [8–10], with $r < 1$. Since the lattice periodicity is bigger than that for the infinite chirality solutions, $r$ is referred to as a ‘redshift’. We checked the validity of the values of $r$ suggested in Ref. [10] and then used them to build the initial conditions. If redshift is not accounted for, the region of stability of blue phases does not change significantly, but the $O_8^-$ phase is not found.

Details of the lattice Boltzmann algorithm used to solve the equation of motion are given in Refs. [15–17]. Calculations were performed on a parallel machine, for a 32x32x32 cubic lattice. This means that, for example, in the case of $O_2$ a cholesteric pitch was discretized into 64 lattice points. Typically, the simulation of one point in the phase space $(\kappa, \tau)$ ran on eight processors and required 8 hours of computational time. Periodic boundary conditions were used throughout. To ensure that equilibrium was reached, we required that the variation in the free energy after 200 iterations of Eq. (4) was smaller than $10^{-4}$ before ending the run. A convenient value of $\Gamma$, ensuring numerical stability and fast computation time, was 0.33775.

The parameters defining the free energy were chosen to match typical values for cholesterics. In what follows the points on the phase diagram will be labelled by their $(\kappa, \tau)$ (as in Ref. [10]) or $(A_0, \gamma)$ values. These can be related straightforwardly via the transformation in Eq. (3).

**IV. RESULTS**

In this Section we report the results obtained for the defect structure of the blue phases, and the equilibrium phase diagram in the vicinity of the isotropic-cholesteric transition. We also consider the dynamics of the defect lines as equilibrium is approached.
A. Defect structure: $O_2$, $O_5$, $O_8^+$ and $O_8^-$

As a first check, we compute the defect structure associated with the cubic blue phases after equilibration. We choose $A_0 = 0.001$ and $\gamma = 2.8$, while the elastic constant $K = 0.01$ for $O_2$, and $K = 0.005$ for $O_5$ and $O_8^{\pm}$. These correspond to a chirality $\kappa = 1.93$ and a reduced temperature $\tau = 4.37$. The resulting disclination line networks are shown in Fig. 1. The tubes in the figure represent regions of the blue phase unit cell in which the order parameter drops below some specified threshold, i.e. they represent disclination lines. The thickness of the tubes is related to the width of the defect cores.

These structures are in good agreement with those obtained in Refs. [10–12]. We note that the structure of the defects depends on the parameters. If $A_0$ or $\gamma$ are increased, i.e. if $\kappa$ decreases, then the width of the disclinations decreases and the drop in order parameter at the defect cores becomes shallower.

We also checked the three-dimensional director field profile and found the presence of distinct regions of double twist separated by the defects shown in Fig. 1, in qualitative agreement with the usual theoretical picture of blue phases [9,10,13].

B. Phase diagram

Next we report results for the free energy of the equilibrated blue phases. In Fig. 2 we show free energy curves for $O_2$, $O_5$, $O_8^\pm$, $O_8^-$ and the isotropic and cholesteric phases for $A_0 = 0.001$ and variable $\gamma$. It can be seen that blue phases appear near the transition to the isotropic phase. As $A_0$ increases, the region of stability of blue phases shrinks. This is in agreement with previous experimental and analytical results in the literature [5,10–12].

In Fig. 3, we show the phase diagram in the $(\kappa, \tau)$ plane which identifies for every point which of the phases, $O_2$, $O_5$, $O_8^{\pm}-$, cholesteric or isotropic, has the minimum free energy. For comparison we show, in the same plane, the phase diagram obtained in Ref. [10] which employed a Fourier expansion of the tensor order parameter $\mathbf{Q}$ around the $\kappa = \infty$ limit.
We stress that the main difference is that in our case we relax the structures (with the disclination network topology suggested in Ref. [10]) by dynamically solving Eq. (4). So the configurations used to construct our phase diagram are actual (in general local) minima of the Landau-de Gennes free energy. In Ref. [10], the configurations found correspond to the free energy minima within a restricted phase space in which the $Q$ tensor expression is constrained to be a sum of spherical harmonics of order $m \leq 2$ with variable coefficients.

Overall, we find qualitative agreement in that (a) the stable phases found (for the parameters investigated here) are $O_2$, $O_5$ and $O_8^-$, (b) $O_5$ appears for high chirality only, and (c) the phase diagram is consistent with the assignment of BP I as $O_8^-$ and of BP II as $O_2$ proposed in [10,12]. However, a few relevant differences should be stressed. First, the region of stability of $O_5$ is shifted to unphysically high values of the chirality $\sim 2$. (Values of $\kappa < 1.2$ are found in cholesterics.) This result is consistent with the observations, which ruled out structures of $O_5$ symmetry from the known blue phases. The region of stability of $O_8^-$ expands and reaches lower chirality values. The critical point below which blue phases are no longer stable is also shifted from $\kappa \sim 0.6$ to below $\kappa = 0.5$ (deeper into the experimentally accessible region). Pleasingly, this leads to the correct order of appearance of BP I and BP II as the chirality is increased (as found in the experiments). This was not achieved before within the Landau-de Gennes framework.

To construct the phase diagram in Fig. 3, we used the values of the redshift from Ref. [10], which were obtained within the approximate framework detailed above. As a check, for a few points in the phase diagram, we equilibrated systems with different redshifts. Plots of free energy versus redshifts for two points in the phase diagram are shown in Fig. 4. At all points we tested we found that the redshift values in Ref. [10] corresponded very closely to the free energy minimum. In this way we feel confident that an extensive calculation taking into account all possible redshifts for all data points, which is numerically extremely expensive, would give a quantitatively very similar phase diagram.

The discrepancy between the phase diagram obtained here and the one given in Ref. [10] show that high order Fourier components of $Q$ are important at least in some regions of the
phase diagram. Indeed the authors of Ref. [10] noted that in a large part of the region where the phase diagrams differ the energies of the various phases are very close. Thus considering a larger variational space could well change the phase boundaries.

**C. Dynamics of the approach to equilibrium**

It is interesting to consider the dynamics of the approach to equilibrium of the blue phases from the infinite chirality initial states. The $O_2$ and $O_8^-$ structures are initially quite far from their equilibrium configurations, while the $O_5$ and $O_8^+$ configurations are closer. This means that the free energy for $O_5$ is lower than that of $O_2$ or $O_8^-$ at the beginning of the simulations. During equilibration, the finite chirality deforms the tensor configurations of $O_2$ and $O_8^-$ via a process which can be suggestively compared to the acquisition of an infinite number of harmonics in the language of [10] and the curves eventually cross. The approach to equilibrium of the free energy was in all cases found to be well represented by an exponential decay to the equilibrated value, with the decay rate playing the role of a relaxation time. Since the transitions are all (weakly) first order this is as expected on general grounds.

The most interesting dynamics of approach to equilibrium is that of $O_8^-$. In this case the initial structure does not closely resemble the equilibrium structure (see Fig. 5). In particular the disclination line along the axis [111] is only partially present. During equilibration, it assembles by the formation of isolated local defects aligned along [111] which then merge into a disclination line. The dynamical evolution was found to be almost independent of the values of $A_0 \neq 0$ and $\gamma$ studied. It would be interesting to follow the evolution of the disclination line experimentally to see whether this effect can be realistic. Calculations are currently underway to check if the same pathway is followed when the full hydrodynamic equations of motion of the liquid crystal are solved.
V. CONCLUSIONS

In conclusion, we have numerically minimised the Landau-de Gennes free energy of a cholesteric liquid crystal and identified the region of stability of the blue phases. It was possible to obtain results for any values of the chirality $\kappa$, that is, for any degree of biaxiality of the tensor order parameter. Our results qualitatively confirm those obtained previously using expansions for large or small $\kappa$. However there are quantitative differences; in particular the blue phases first appear at a value of $\kappa \sim 20\%$ smaller than in the approximate minimisations. Also, it is interesting to note that the full numerical solution presented here produces for the first time the correct order of appearance of BP I and BP II at low chiralities, while the $O_5$ phase, which was not observed in experiments, is relegated to unphysical values of the chirality. We finally followed the approach to equilibrium. In the case of $O_5\overline{5}$ the disclination network assembles during the equilibration via an intermediate state in which aligned isolated defects appear and then join to form the disclination line along the cube lattice diagonal.

Note that in two rather recent papers [18,19], it was found that adding fluctuations to the Landau-de Gennes free energy could render the phase diagram more realistic in that e.g. the region of stability of $O_5$ was restricted. Here we find a similar result by an exact minimisation of the mean field free energy without including fluctuations.

Finally, our approach can be generalised to study the effect of an electric field on the phase diagram as well as the dynamics of the switching of a blue phase device, such as the one proposed in Ref. [7]. Further work is underway along these lines.

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REFERENCES

[1] P. G. de Gennes and J. Prost, *The Physics of Liquid Crystals, 2nd Ed.*, Clarendon Press, Oxford (1993).

[2] S. Chandrasekhar, *Liquid Crystals*, Cambridge University Press, (1980).

[3] E. Grelet, S. Fraden, *Phys. Rev. Lett.* **90**, 198302 (2003).

[4] D. C. Wright, N. D. Mermin, *Rev. Mod. Phys.* **61**, 385 (1989).

[5] M. Marcus, J. W. Goodby, *Mol. Cryst. Liq. Cryst. Lett.* **72**, 297 (1982).

[6] W. Y. Cao, A. Munoz, P. Palffy-Muhoray et al., *Nat. Mater.* **1**, 111 (2002).

[7] H. Kikuchi, M. Yokota, Y. Hisakado et al., *Nat. Mater.* **1**, 64 (2002).

[8] R. M. Hornreich, S. Shtrikman, *Phys. Rev. A* **24**, 635 (1981).

[9] H. Grebel, R. M. Hornreich, S. Shtrikman, *Phys. Rev. A* **28**, 1114 (1983); *Phys. Rev. A* **28**, 2544 (1983).

[10] H. Grebel, R. M. Hornreich, S. Shtrikman, *Phys. Rev. A* **30**, 3264 (1984).

[11] S. Meiboom, M. Sammon, W. F. Brinkmann, *Phys. Rev. A* **27**, 483 (1983).

[12] S. Meiboom, M. Sammon, D. W. Berreman, *Phys. Rev. A* **28**, 3553 (1983).

[13] S. Meiboom, J. P. Sethna, P. W. Anderson, W. F. Brinkman, *Phys. Rev. Lett.* **46**, 1216 (1981).

[14] A. N. Beris, B. J. Edwards, *Thermodynamics of Flowing Systems*, Oxford University Press, Oxford (1994).

[15] C. Denniston, E. Orlandini, J. M. Yeomans, *Europhys. Lett.* **52**, 481 (2000); *Phys. Rev. E* **63**, 056702 (2001).

[16] C. Denniston, D. Marenduzzo, E. Orlandini, J. M. Yeomans, *Phil Trans. R. Soc. Lond.*
A 362, 1745 (2004).

[17] D. Marenduzzo, E. Orlandini, J. M. Yeomans, Phys. Rev. Lett. 92, 188301 (2004).

[18] J. Englert, L. Longa, H. Stark, H.-R. Trebin, Phys. Rev. Lett. 81, 1457 (1998).

[19] J. Englert, L. Longa, H. Stark, H.-R. Trebin, Phys. Rev. E 61, 2759 (2000).
FIGURES

FIG. 1. Defect structure where $\gamma = 2.80$ and $A_0 = 0.001$ for (a) $O_2$, (b) $O_5$, (c) $O_8^+$ and (d) $O_8^-$. 

FIG. 2. Free energy of $O_2$, $O_5$, $O_8^+$, $O_8^-$ and the cholesteric helix as a function of $\gamma$ for $A_0 = 0.001$. 
FIG. 3. Left, phase diagram in the \((\kappa, \tau)\) plane obtained numerically (this work). Right, phase diagram from Ref. [10].

FIG. 4. Plot of the free energies (simulation units) of \(O_2\), \(O_8^+\), \(O_8^-\) for two points in the \((A_0, \gamma)\) plane ((0.006,3) for the top three curves and (0.002,3.5) for the bottom three). Dashed lines are quadratic fits. Squares and stars show the numerical minimum and the one found in Grebel et al. [10] respectively.
FIG. 5. Evolution of the defect structure (from left to right) for $\gamma = 2.80$ and $A_0 = 0.001$, for the $O_8^-$ configuration. The initial configuration is stable for $A_0 = 0$. 