Chapter 4

Local and nonlocal properties of the isotropic-nematic interface

In this chapter we discuss applications of the numerical methodology presented in the previous chapter to problems arising in the study of the isotropic-nematic interface. We solve the GLdG equations in equilibrium to obtain the profile of the nematic orientation tensor at the interface as well as in the bulk. We calculate the conformation of the isotropic-uniaxial nematic interface with different anchoring conditions imposed on the director asymptotically distant from the interface. Using our MOL scheme, we test the validity of the “de Gennes ansatz” for the isotropic-uniaxial interface, considering all degrees of freedom of the nematic orientation tensor, unlike previous work. These results demonstrate the validity of the de Gennes ansatz in a well-defined limit of the Landau-Ginzburg-de Gennes theory and specifically illustrates regimes when this ansatz breaks down [57].

In the following section, using our accurate spectral collocation scheme, we show how including elastic anisotropy leads to a biaxial interface with planar anchoring of the nematic director at the nematic boundary. In subsequent sections, by extending our spectral scheme to deal with an arbitrary anchoring of the nematic director, we show how oblique nematic anchoring breaks the local property of the interface, yielding a smooth profile of the tilt angle far from the interface.

We conclude the chapter with a discussion of the effects of thermal fluctuations on the roughness of the interface profile. This is, to our knowledge, the first GLdG calculation of the properties of the noisy isotropic-nematic interface. Such calculations, in the absence of ad-hoc approximation of the nematic equations have not been previously performed in the literature.

4.1 Introduction

Liquid crystalline states of matter provide a useful testing ground for statistical mechanical theories of interface structure, since a variety of ordered phases can be accessed in experiments and computer simulations. The structure of the isotropic-nematic (I-N) interface presents a simple example of how interfacial order can differ radically from order in the coexisting bulk phases, since biaxial order is generically expected at the interface even if the
stable ordered phase is purely uniaxial.

Suppose we consider a nematic strip in the \( x-z \) plane sandwiched between an isotropic medium on both sides. The variation can occur in the \( z \) direction while translational symmetry excludes variation along the \( x \) direction. The free energy of the nematic strip per unit length consists of contributions both from the bulk term and the surface energy cost for the interface, given as

\[
\frac{\mathcal{F}}{L_z} = -aL_x \Delta F + L_x \sigma, \tag{4.1}
\]

where \( a \) is the stripwidth, \( L_x \) is the length of the interface, \( \Delta F \) is the difference in the free energy density of the nematic to isotropic phase and \( \sigma \) is the line tension of the interface. At any temperature below or above coexistence, \( \Delta F \neq 0 \). Depending on the sign of \( \Delta F \), the interface moves with a velocity \( v \) resulting in either an isotropic medium or a nematic medium spanning the system size \([56]\). At coexistence, \( \Delta F = 0 \) and \( v = 0 \). The only contribution to the free energy comes from the surface term and the planar interface is stable in this regime.

The study of the isotropic-nematic interface within the framework of a Landau-Ginzburg description was initiated in an insightful paper by de Gennes \([23]\). To render the problem analytically tractable, de Gennes made a specific assumption regarding the variation of the components of the order parameter across the interface. For an infinitely extended interface where, by homogeneity, variations perpendicular to the interface alone are allowed, de Gennes assumed that the only quantity which changed across the interface was the uniaxial strength of ordering \( S \). In the de Gennes ansatz, there is no biaxiality and no variation of the director across the interface. This reduces the nematic problem with five degrees of freedom to a more analytically manageable problem involving only a single degree of freedom. The variation of the ordering strength \( S \) along the coordinate \( z \) normal to the interface located at \( z_0 \) can then be obtained analytically as

\[
S(z) = S_c \left( 1 - \tanh \frac{z - z_0}{w} \right), \tag{4.2}
\]

where \( w = \sqrt{2}/S^* \) is the non-dimensional interfacial width, \( S^* = S/S_c \) being the non-dimensional strength of ordering and \( S_c \) the value at coexistence.

The de Gennes ansatz is exact in the absence of elastic anisotropy. However, the description of the interface in the presence of such anisotropy poses a formidable analytic and numerical problem, since the partial differential equations for the five independent components of \( Q_{\alpha \beta} \) contain non-linear couplings, while \( Q_{\alpha \beta} \) is itself constrained by symmetry and the requirement that its trace vanish.

Popa-Nita, Sluckin and Wheeler (PSW) \([57]\) studied the I-N interface incorporating elastic anisotropy in the limit of planar anchoring, adapting a parametrization introduced by Sen and Sullivan \([64]\). These authors neglected the twist distortion in their formulation and assumed that the director was contained always in a single plane (say \( x-z \) plane). This defines the \([nlm]\) triad through a single angle, called the local tilt angle, and defined as \( \theta = \cos^{-1}(k \cdot n) \). This reduces the five independent degrees of freedom of the problem to three. In the PSW parametrization, the principal axes of \( Q_{\alpha \beta} \) remain fixed in space, and the problem reduces to the solution of two coupled non-linear partial differential equations
4.1. Introduction

Figure 4.1: Panel (a) depicts the interface geometry and the coordinate system used in our calculations. The nematic director makes an angle $\theta$ with the $z$ axis. It can be chosen to vary between 0 (homoeotropic anchoring) and $\pi/2$ (planar anchoring). The isotropic phase is favoured through boundary conditions, as $z \to -\infty$, whereas the nematic phase is favoured for $z \to \infty$. The plane of the interface is the $x-y$ plane, shown by $ABCD$ in the figure, whereas the director is confined to the $EFGH$ plane as shown. The origin is denoted by $O$. In panel (b) we show a numerical realization of the interface neglecting thermal fluctuations and with a planar anchoring condition. The nematic strip of width 128 is sandwiched between isotropic phases with periodic boundaries.
in the dimension perpendicular to the interface. These equations represent the variation of the amplitude of uniaxial and biaxial ordering across the interface.

PSW obtained numerical solutions for the variation of $S$ and $T$ across the interface and showed that the solutions of these equations exhibited biaxiality in a region about the interface. The uniaxial order parameter ($S$) was adequately represented by a tanh profile, as in the original calculation of de Gennes, while the biaxial order parameter ($T$) exhibited more complex behaviour, peaking towards the isotropic side and with a trough on the nematic side. The biaxial profile was also shown to have a long tail towards the isotropic side, a feature hard to anticipate on physical grounds. For a general anchoring condition this parametrization breaks down, as is obvious from the fact that the order parameter has, in general, five independent components.

We begin with the GLdG expansion of the free energy for a general $Q_{\alpha\beta}$

\[
\mathcal{F} = \int dz dx_\perp \left[ \frac{1}{2} A \text{Tr} Q^2 + \frac{1}{3} B \text{Tr} Q^3 + \frac{1}{4} C (\text{Tr} Q^2)^2 
\right. \\
\left. + \frac{1}{2} L_1 (\partial_\alpha Q_{\beta\gamma})(\partial_\alpha Q_{\beta\gamma}) + \frac{1}{2} L_2 (\partial_\alpha Q_{\alpha\gamma})(\partial_\beta Q_{\beta\gamma}) \right]. 
\] (4.3)

where all the constants are having their meaning as defined previously. The variation happens in $z$ direction while the interface is in the plane $\perp$ to $z$ axis. We choose $A = B^2/27C$, thus enforcing phase coexistence between an isotropic and uniaxial nematic phase [32]. The interface is taken to be flat and infinitely extended in the $x-y$ plane. The spatial variation of the order parameter only occurs along the $z$ direction [64].

In the case of planar anchoring, the ordering at infinity is purely uniaxial and taken to be along the $x$ axis. In this case, as shown by Sen and Sullivan, uniaxial and biaxial order vary only with $z$ and the principal axes of the $Q$ tensor remain fixed in space. The form of $Q$ is then

\[
Q = \begin{pmatrix} S & 0 & 0 \\ 0 & -\frac{1}{2}(S-T) & 0 \\ 0 & 0 & -\frac{1}{2}(S+T) \end{pmatrix}. 
\] (4.4)

We solve the nematic equations in equilibrium, which are

\[
(A + C \text{Tr} Q^2) Q_{\alpha\beta}(x,t) + B Q_{\alpha\beta}(x,t)^2 = L_1 \nabla^2 Q_{\alpha\beta}(x,t) + L_2 \nabla_\alpha(\nabla_\gamma Q_{\alpha\gamma}(x,t)). 
\] (4.5)

These results from the condition $\delta \mathcal{F}/\delta Q = 0$ constrained to the condition of vanishing trace and symmetry of $Q$. We employ the change in basis $Q \rightarrow T$ as defined in Eq.(1.13), so that the variational equations take the form,

\[
(A + C \text{Tr} Q^2) a_i + B T^i_{\alpha\beta} Q_{\alpha\beta} = L_1 \nabla^2 a_i + L_2 T^i_{\alpha\beta} T^j_{\beta\gamma} \partial_\alpha \partial_\gamma a_j. 
\] (4.6)

The complete set of equations with the boundary conditions are displayed in Appendix B.

We solve this set of equations, employing proper boundary conditions (planar, homeotropic and oblique director anchoring) to study the problems discussed in the following sections. Anchoring of the director at the isotropic-nematic interface can also be imposed through an
4.2 Verification of de Gennes ansatz

We have verified the remarkable de Gennes ansatz through a direct numerical solution. In our numerical calculations, a strip of nematic interface is sandwiched between two isotropic domains with periodic boundary conditions. The system was allowed to relax to the minimum of the free energy. The parameters were chosen such that the width $w \gg \Delta z = 1$, ensuring that discretization errors were kept to a minimum.

The resulting profiles for the variation of $S$ and $T$ are shown in Fig. (4.2). The values obtained for $T$ are consistent with de Gennes’ assumption of vanishing biaxiality. The variation of $S$ at each of the two isotropic-nematic interfaces were fitted, using the least-squares method, to the analytical profile, with the saturation value of the order $S_c$, the location of the interface $z_0$ and the interface width $w$ as fitting parameters. As shown in the inset to Fig. (4.2), fitted values of $w$ agree remarkably well with the analytic result for a range

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<th>Figure</th>
<th>$A$</th>
<th>$B$</th>
<th>$C$</th>
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<th>$L_1$</th>
<th>$L_2$</th>
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<td>$-0.5$</td>
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<td>$B^2/27C$</td>
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Table 4.1: Numerical parameters in the Landau-de Gennes theory used to construct the figures.

inclusion of a term proportional to $\zeta Q_{\alpha\beta} \phi_{\alpha} \phi_{\beta}$ in the free energy functional, where $\zeta$ represents the strength and $\phi_{\alpha\beta}$ is a quenched field following the interface structure. However in this study, we impose the director anchoring from the degree of anisotropy in the elastic constants as shown in the subsequent sections. In the next section, we verify “de Gennes ansatz” in a particular limit of the GLdG theory. The next section is devoted for the discussion of the nature of I-N interface with planar anchoring of the nematic director at the nematic boundary. We discuss the effect of oblique anchoring of the nematic director in the subsequent section. The GLdG parameters used for the calculations are highlighted in Table 4.1.
Figure 4.2: Variation of the degree of alignment (S) and biaxiality (T) across the nematic - isotropic interface with planar anchoring. Symbols represent numerical data, solid curves are the de Gennes ansatz (4.2). Nematic strip width = 256. The inset shows the variation of the interfacial width with the elastic constant $L_1$. The expected quadratic variation is accurately reproduced.

of parameter values. The agreement is accurate to within a fraction of a percent. Similar results were obtained for the saturation value of the order parameter. This benchmark also clearly demonstrates the accuracy of the MOL scheme in reproducing the equilibrium limit of Eq.(1.34).

The de Gennes ansatz also predicts that the energies of planar and homeotropic anchoring are identical when elasticity is isotropic ($L_2 = 0$). We compared the value of the free energies of the interface for both planar and homeotropic anchoring of the director. To machine precision, these answers are identical. Our results for this problem represent the first direct verification of the de Gennes ansatz retaining all degrees of freedom of the orientational tensor.

4.3 Isotropic-nematic interface with planar anchoring

To study the effect of different nematic director anchoring conditions to the I-N interface, we use the spectral collocation technique, described in the previous chapter, to solve the variational equations 4.6. The polynomial interpolant is constructed so as to satisfy Dirichlet boundary conditions. Though the physical problem is for an unbounded interval, our numerical approximation of a bounded interval gives excellent results since all variation in the order parameters is restricted to the region proximate to the interface. de Gennes in his calculation, based on energetic arguments showed that for $L_2 > 0$ planar anchoring was the stable interface conformation while homeotropic anchoring was the most probable
4.3. Isotropic-nematic interface with planar anchoring

Figure 4.3: Convergence of the uniaxiality parameter $S$ across the nematic-isotropic interface with planar anchoring. The inset shows the convergence of biaxiality parameter $T$. The convergence is achieved for the polynomials higher than $N = 96$, which is been shown as a single curve for $N = 128, 160$ and $192$.

conformation for $L_2 < 0$.

4.3.1 Benchmarking the spectral collocation technique

To reduce the error to a minimum, we perform a systematic check of the nematodynamic equations with incorporating an increasing number of Chebyshev polynomials. We choose $L_1 = 10^{-6}$ in our numerics and obtain $L_2$ from our choice of $\kappa$. The spectral collocation reduces the nematodynamic differential equations (A.1) to non-linear algebraic equations. We solve them using a relaxation method from a well-chosen initial condition, relaxing till the differential change in successive iterations is less than $10^{-5}$. Spectral convergence to machine accuracy is obtained by retaining 128 Chebyshev modes, as we have checked by an explicit calculation shown in Fig. 4.3. To compare with analytical and density functional results, the solution at the Chebyshev nodes is interpolated using barycentric interpolation (which is a spectrally accurate global polynomial interpolation) without compromising spectral accuracy.

4.3.2 Local biaxiality at the interface

The central results are depicted in Fig. 4.4. The analytical profile of the biaxiality $T$ in the low $\kappa = L_2/L_1$ limit is due to Kamil et al. [35], which we plot together with the previous analytical profile due to PSW [57]. In Fig. 4.4(a), in the main panel, we plot the biaxiality $T$ for these two analytical approaches and our spectral data. The analytic form of $T$ fits well to the spectral data, particularly away from the main peak, yielding essentially exact agreement deep into the isotropic and nematic sides. The PSW approximation overestimates the peak
Figure 4.4: Uniaxial and biaxial profiles across the nematic - isotropic interface with planar anchoring. In (a) (main panel), a comparison of the T profile obtained from the analytical expression by Kamil et al., PSW and our spectral data is plotted. The inset shows that of the uniaxial (S) profile for this case. In (b) (main panel), we show the uniaxial profile and the inset for the biaxial profile with increasing $\kappa$. In (c), we show the increasing biaxiality of the biaxial parameter $\omega$, defined in Eq. (1.23) with $\kappa$. 
4.4 The isotropic-nematic interface with oblique anchoring

value, and also differs sharply in relation to the numerical data deep into the isotropic side. The inset to Fig. 4.4(a) shows the uniaxial (S) profile for this case. In Fig. 4.4(b) we show the profile obtained with our method for S and T with increasing \( \kappa \). Benchmarking this part is outside the scope of an analytical treatment.

4.4 The isotropic-nematic interface with oblique anchoring

Nematic ordering is strongly influenced by confining walls and surfaces, which impose a preferred orientation or "anchoring condition" on the nematic state. Such a preferred orientation yields an anchoring angle, defined as the angle made by the director in the immediate neighbourhood of the surface with the surface normal. Anchoring normal to the surface is termed as homoeotropic, whereas anchoring in the plane of the surface is termed as planar. The intermediate to this two cases is termed as oblique anchoring.

As is the case with surfaces, the interface between a nematic and its isotropic phase can also favour a particular anchoring. The problem of interface structure for the nematic is particularly interesting since it illustrates how the structure in the interfacial region can differ substantially from structure in the bulk. The previous section demonstrated that a region proximate to the interface could exhibit biaxiality within the LGdG theory, even if the stable nematic phase is purely uniaxial, provided planar anchoring is enforced at the nematic boundary. Such biaxiality is absent if the anchoring is homoeotropic \[ 23 \]. These two limits, of homoeotropic and planar anchoring, lead to interface profiles of S and T which vary only in the vicinity of the interface, as well as orientations which are uniform across the interface \[ 23 \].

An interesting question is whether an oblique nematic anchoring can be stable at the interface between a bulk uniaxial nematic and its isotropic phase within GLdG theory. Suppose we introduce boundary conditions that impose a specified oblique orientation asymptotically within the nematic phase, where the magnitude of the order parameter is saturated. The question, then, is whether such an imposed orientation is relaxed to a preferred value in the vicinity of the interface. The difficulties with this problem stem from the fact that changes in the local frame orientation on the nematic side of the interface come with an elastic cost arising out of nematic elasticity. This is an effect sensitive, in principle, to system dimensions, since gradients can be smoothed out by allowing the changes to occur over the system size. While this cost can be reduced by suppressing the order parameter amplitudes in regions where order parameter phases vary strongly, the precise way in which this might happen, if at all, is an open question.

PSW \[ 57 \] studied this problem numerically within a GLdG approach, using a set of variables \( \eta_s \) and \( \mu_s \) introduced by Sen and Sullivan in ref. \[ 64 \]. These variables are combinations of the variables S, T and \( \theta \). Although the focus of their study was the emergence of biaxiality at the interface with a planar anchoring condition, PSW remarked that if the asymptotic orientation of the director in the nematic phase was set to any value other than 90° (planar anchoring) or 0 (homoeotropic anchoring) for large \( z \), then \( \eta_s \) and \( \mu_s \) approached this value with non-zero slope. PSW thus concluded that there could be no stable anchoring if the orientation of the director in the nematic phase was neither planar nor homoeotropic,
but oblique. The precise nature of the resulting state obtained upon applying an oblique anchoring condition was not addressed by PSW [56, 57].

Density functional calculations on hard-rod systems using Onsager’s theory applied to the free isotropic-nematic interface indicate that the minimum surface free energy is obtained when the rods lie parallel to the isotropic-nematic interface, the case of planar anchoring [47, 3]. Molecular simulations of a system of hard ellipsoids, in which an anchoring energy fixes the director orientation in the nematic phase at a variety of angles, indicate that the isotropic-nematic interface favours planar anchoring. These simulations, and a mean-field calculation based on the Onsager functional, find that the angle profile is approximately linear as one moves away from the boundary condition imposed by the wall at one end of the simulation box [76, 71]. These results, in particular concerning the stability of planar anchoring, are consistent with those from other treatments [7, 19, 18, 2, 72].

However, several other papers indicate specific regimes in which homoeotropic or oblique anchoring may be stable. Moore and McMullen [52] numerically evaluate the inhomogeneous grand potential within a specific approximation scheme finding that planar anchoring is preferred at the interface for long spherocylinders, but oblique or homoeotropic anchoring may be an energetically favourable alternative for smaller aspect ratios. Holyst and Poniewierski study such hard spherocylinders in the Onsager limit, noting that oblique anchoring is favoured over a considerable range of aspect ratios [34]. Finally, experiments provide evidence for both oblique [28] and planar anchoring [41], with electrostatic effects possibly favouring oblique anchoring.

We study the isotropic-nematic interface within GLdG theory in the case where an oblique anchoring condition is imposed on the nematic state far from the location of the interface [36]. The analytical treatment to this problem is by Kamil et al which is satisfactory in a limiting case of small $\kappa$ [36]. For a flat interface, the components of $Q$ can depend only on the coordinate perpendicular to the interface. We work at phase coexistence, imposing boundary conditions fixing the isotropic phase at $z = -\infty$ and the nematic phase at $z = \infty$. The components of $Q$ as $z \to \infty$ are chosen so that $S$ is fixed to its value at coexistence $S_c$, while the axis of the nematic is aligned along a specified (oblique) direction. The coexisting states are separated by an interface in which order parameters rise from zero on the isotropic side of the interface to saturated, non-zero values on the nematic side. Since the two free energy minimum states are degenerate in the bulk, the position of the interface is arbitrary and can be fixed, for concreteness, at $z = 0$ in the infinite system.

However, there are subtleties. Provided all components of $Q$ vary substantially only in the neighbourhood of the interface, the interface can be located through several, largely equivalent criteria. However, if variations of $Q$ are not confined to a region proximate to the interface but depend on the system size $L$ irrespective of how large $L$ is, the very isolation of an interface from the bulk is ill-defined. As indicated earlier, it is this situation which obtains in the case of oblique anchoring and the $L \to \infty$ limit must be taken with care.

We summarize the results of the study: A numerical minimization of the GLdG free energy which imposes a specific oblique anchoring condition on the system deep into the nematic while fixing the interface location at the origin shows that the elements of $Q$ vary with space even far away from the interface, albeit slowly. Only in the limit of homoeotropic
4.4. The isotropic-nematic interface with oblique anchoring

Figure 4.5: Panel (a) shows the variation of the uniaxial degree of alignment ($S$) and biaxiality ($T$) across the nematic - isotropic interface for oblique nematic anchoring. Panel (b) shows that of the local tilt angle $\theta$. Panel (c) shows the variation of the local tilt angle across the interface for an oblique nematic anchoring fixed to $\theta = \pi/4$ at the nematic boundary. Panel (d) shows the variation of the local tilt angle with different values of the elastic constant and the extrapolation of the data to account for the system size $\rightarrow \infty$ or $L_1 \rightarrow 0$ limit. 128 Chebyshev polynomials are taken for the numerics.
or planar anchoring is the variation of $Q$ confined to a finite region. This variation in the case of oblique anchoring can, however, be split into hydrodynamic and non-hydrodynamic components. Generically, the variation of the non-hydrodynamic components, such as the magnitudes of $S$ and $T$, are confined to a finite region, independent of the system size $L$, if $L$ is large enough. However, the orientation of the nematic director varies in space: if the asymptotic value of the nematic order parameter at $L$ represents uniaxial ordering along an oblique axis, the director orientation interpolates linearly between either $\pi/2$ preferred at the location of the interface (planar anchoring) or $0$ (homeotropic anchoring), and the value imposed by the boundary condition at $L$. Whether planar or homeotropic anchoring is preferred at the interface depends on the sign of the anisotropic elastic term, as initially shown by de Gennes [23].

Our results are broadly consistent with the qualitative observations of PSW, but provide a detailed quantitative analysis in the case of oblique anchoring. In the limit that $L \to \infty$, the total energy cost for elastic distortions of the nematic field $\sim \int (\nabla \theta)^2 dz \sim 1/L$, thus vanishing in the thermodynamic limit. Thus, the isotropic-nematic interface with an oblique anchoring constraint imposed on the nematic side can be regarded as being marginally stable, as opposed to unstable, provided the thermodynamic limit is taken with care.

### 4.4.1 Non-locality of the tilt angle with $\kappa > 0$

Stability imposes the requirement that $6 + \kappa > 0$ so that the tangential coherence length is a positive quantity. In this section we explore the consequences of a positive value of $\kappa$.

The results of our findings are summarized as follows: In Fig.[4.5(a)] we plot the $S$ and $T$ profile for the oblique anchoring angles $0, \pi/8, \pi/4, 3\pi/8$ and $\pi/2$. The $T$ profile shifts origin as the anchoring is shifted from homeotropic to planar. This is also reflected in the profile of $S$ shown in the inset. We also recover the vanishing biaxiality in the homeotropic anchoring case, as first obtained by de Gennes [23]. In Fig.[4.5(b)], we show the monotonic increase in the slope of the local tilt angle $\theta$ as the interface is approached from the nematic boundary and also the nematic anchoring is tilted from homeotropic ($\theta = 0$) to planar ($\theta = \pi/2$). As the director on the isotropic side of the interface is a undefined quantity, we plot $\theta$ with a straight line for ease. The slope vanishes only when the true thermodynamic limit $L \to \infty$ is achieved. The interface anchoring is smoothly approached from the anchored nematic boundary in a linear way. In Fig.[4.5(c)], for a fixed anchoring of the nematic director at the boundary as $\theta = \pi/4$, how the anchoring angle behaves at the interface as the elastic constant $L_1$ is decreased, which is effectively to increase the system size of the problem. Finally we show in Fig.[4.5(d)] the increment of the anchoring angle with the decrement of $L_1$. We mention that the system size is fixed from the boundary between [-1,1] and decrement of the elastic constant $L_1$ effectively increases the effective correlation length of the problem. In Fig.[4.5(d)] we also plot the polynomial extrapolation of the data that reflects the director anchoring at the $L \to \infty$ limit of the problem, i.e. the $L_1 \to 0$. However the extrapolation is affected severely with only a few points and thus yields a value of $\theta < \pi/2$. 
4.5. Fluctuation of the I-N interface

The nature of the isotropic-nematic phase in the presence of thermal fluctuation has only been previously addressed using molecular dynamics simulations [62]. So far to our knowledge, the nature of the interface described from a fluctuating Ginzburg-Landau theory is not previously addressed.

We perform our numerics with a nematic strip of size 128 sandwiched between isotropic phases with periodic boundaries on a 256$^2$ lattice. At coexistence, defined in the absence of fluctuations, we see a successive collapse of the uniaxial nematic phase with a local melting of

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1 We show the T profile for only planar and homeotropic anchoring due to non-convergence of the profiles in the computational time for intermediate anchoring angles.
the interface after certain period in time. Slightly below coexistence, we see an expansion of the fluctuating interface without melting of the interface which finally excludes the isotropic fluid phase completely.

In Fig. (4.7), we exhibit the calculated interface at time \( t = 6 \times 10^3 \), with the isotropic phase in the left and the nematic phase on the right. Only one side of the interface is shown. Colours indicate the values of the order parameter, with zero on the left (blue colour) and nematic saturation values on the right (yellow colour). The local orientation field is also shown, indicating alignment in the nematic state perpendicular to the interface. The roughening of the interface by noise-induced capillary excitations, an effect absent in the conventional mean field, zero noise treatment of this problem can be clearly seen. The capillary fluctuations add to the interface width computed within a mean-field treatment of the GLdG functional. They also modify the surface tension in nontrivial ways \([62]\).

4.6 Conclusion

In this chapter we have discussed the conformation of the isotropic-uniaxial nematic interface with different anchoring conditions imposed on the director, in the presence and in the absence of elastic anisotropy terms. We obtain the profile of the nematic orientation tensor at the interface as well as in the bulk. We show in the limit \( \kappa = 0 \), de Gennes ansatz for uniaxial interface is valid. In the limit \( \kappa \neq 0 \), the interface become biaxial, with planar anchoring of the nematic director at the nematic boundary. We the showed how oblique
nematic anchoring breaks the local property of the interface, with a smooth profile of the tilt angle far from the interface. Finally, we demonstrate the effect of thermal fluctuation on the roughness of the interface profile.