A model liquid crystal cell in an RC circuit

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Abstract

A nematic liquid-crystal cell subject to an electric field created by electrodes held at constant potential is modeled as a variable capacitor in an RC circuit. The state of the system is characterized in terms of the director field in the cell and the charge on the electrodes. A dynamical system is developed that couples director dynamics in the cell (with no fluid flow) and charge dynamics in the circuit. The dynamical equations are derived from expressions for the total potential energy of the system and a dissipation involving a single rotational viscosity for the director plus Joule heating associated with current in the circuit. An effort is made to quantify effects, in particular the widely differing time scales for the processes involved, and numerical illustrations are given. The exercise illuminates aspects of the modeling of equilibrium states of such a system.

Keywords: nematic liquid crystal, electric field, Oseen-Frank model, RC circuit

1 Introduction

We are motivated by a desire to understand better the dynamical stability of equilibria of a nematic liquid crystal in an electric field created by electrodes held at constant potential. As modeled in the Oseen-Frank macroscopic continuum theory, the free-energy functional that governs the coupled equilibrium states of the liquid crystal and the electric field can, in the simplest cases, be expressed in the form

$$\mathcal{F}[n, U] = \int_{\Omega} \left[ W_e(n, \nabla n) - \frac{1}{2} \epsilon(n) \nabla U \cdot \nabla U \right] \, dV,$$

(1)

Here $\mathbf{n}$ is the director field (unit-length vector field), $U$ the electric potential (related to the electric field via $\mathbf{E} = -\nabla U$), $\Omega$ the domain of the liquid crystal cell, $W_e$ the density of distortional elastic energy, and $\epsilon$ the dielectric tensor. These terms are characterized more carefully in the next section. The tensor $\epsilon$ is symmetric positive definite, and as a result, the problem has an intrinsic “minimax” nature to it, with locally stable equilibria locally minimizing with respect to $\mathbf{n}$ but maximizing with respect to $U$. The assessment of local stability is well understood from a variational point of view, studied in [8]. However, the
negative definiteness of $F$ with respect to $U$ causes confusion about how to assess stability from a dynamical point of view. The source of this confusion, as we shall see, comes from the modeling assumptions that must be made in order to put the free energy in the form above. In particular, one must assume either a static electric field or an electric field that adjusts instantaneously to changes in the director field in order for (1) to be valid.

The dynamics of such a system can be modeled at different levels of fidelity. A director field that is evolving in time will have associated with it fluid flow in the cell, changes in the local electric field (caused by changes in the dielectric tensor), and changes in the capacitance of the cell (again caused by the changes in the dielectric tensor), which will in turn cause changes in the charge distributions on the electrodes. Hydrodynamics is often of secondary importance (and ignoring it greatly simplifies matters); so we shall assume no fluid flow. In many cases, the time scale for director dynamics is orders of magnitude slower than the time scales for the electric field and circuit dynamics; so a common modeling approximation is to assume that both the electric field and the charge distributions on the electrodes adjust instantaneously to any changes in the director field. This leaves a reduced free energy that is a functional of $n$ only, which makes the “minimax problem” go away. The equilibrium Euler-Lagrange equation for the reduced model is nonlocal, however—the electric field at a point depends on the director field everywhere—though the assessment of stability is “normal,” in that locally stable equilibrium director fields are local minimizers of the reduced free energy.

There are, however, experiments involving “fast switching” (motivated by potential applications for light modulators and the like) in which the time scale for director reorientation is comparable to the time scale for circuit dynamics—see, for example, [9] [11] [21]. There are, in fact, experiments in which the circuit dynamics are a limiting factor [1] [14]. The time scale for the evolution of the electric field, on the other hand, comes from the time-dependent Maxwell equations and is invariably several orders of magnitude faster than any other macroscopic time scale present. We examine these issues more carefully in §4.6.

Here then we assume that the electric field adjusts instantaneously to the director field, but we model faithfully the coupling between the dynamics of the director field and those of the charge distribution. The modeling highlights the role of the voltage source in giving rise to the troubling minus sign in the free energy in (1) above and the assumptions that must be made in order to put the free energy in that form. Also, the coupling between director dynamics and circuit dynamics introduces an additional mechanism for energy dissipation: Joule heating due to current in the circuit.

We choose a “textbook” model system for illustration (a splay-Fréedericksz cell) so that all formulas can be worked out explicitly and are not too cumbersome. Several of our results apply to more general situations, and we try to indicate this at appropriate points. The model problem, free energy, and equilibrium equations are presented in §2. There, both the coupled formulation (in terms of $n$ and $U$) and the reduced formulation (in terms of $n$ only) are discussed. The basic equations characterizing RC circuits are reviewed in §3. In §4, the linkage is made between the state of the director field in the cell and the state of the electric circuit, with a combined potential energy and dissipation function and resulting coupled dynamical system. A simple numerical illustration of the coupled dynamics is given in §5, and what conclusions can be drawn are discussed in §6.
Figure 1: Model problem. Figure 1a: electric-field splay-Fréedericksz-geometry cell (geometry, coordinate system, ground state) as a capacitor in an RC circuit, figure 1b. The liquid crystal film is confined to \(0 < z < d\). Strong anchoring is assumed on \(z = 0\) and \(z = d\), and the liquid-crystal director is assumed to remain in \(\text{span}\{e_x, e_z\}\). RC circuit parameters: resistance \(R\), capacitance \(C\), voltage \(V\), charge \(Q\) (upper electrode +, lower electrode −), current \(I\) (positive direction indicated).

2 Model and equilibrium equations

For a concrete realization of the ideas explored here, we consider a nematic liquid crystal cell in the splay-Fréedericksz geometry (as depicted in figure 1a) subject to an electric field created by electrodes held at constant potential by a voltage source. In devices, the voltage source is usually just a battery, while in experiments, the electromotive force could come from a variable power supply. The system is modeled using the Oseen-Frank macroscopic continuum theory \cite{4, Ch. 3}, \cite{19, Ch. 2}, \cite{22, Ch. 3}. The lateral dimensions of the cell are assumed to be much larger than the cell gap, enabling us to treat all fields as uniform in \(x\) and \(y\) (the coordinates in the lateral directions), with spatial dependence only on the \(z\) coordinate (the coordinate across the cell gap)—thus we ignore the influence of fringe fields and effects near the edges of the cell. We assume strong anchoring conditions and further assume that the director \(\mathbf{n}\) remains in the \(x\)-\(z\) tilt plane:

\[
\mathbf{n} = n_x e_x + n_z e_z = \cos \theta e_x + \sin \theta e_z, \quad \theta = \theta(z).
\]

The free-energy functional will contain contributions from distortional elasticity plus terms associated with the electric field. The elastic part has the form

\[
\mathcal{F}_e[\mathbf{n}] = \int_{\Omega} W_e(\mathbf{n}, \nabla \mathbf{n}) \, dV = A \int_0^d W_e(\mathbf{n}, \partial_z \mathbf{n}) \, dz,
\]

where \(\Omega\) is the domain of the cell, \(A\) the \(x\)-\(y\) cross-section area, \(d\) the cell gap, and

\[
2W_e = K_1 (\text{div} \mathbf{n})^2 + K_2 (\mathbf{n} \cdot \text{curl} \mathbf{n})^2 + K_3 |\mathbf{n} \times \text{curl} \mathbf{n}|^2
= K_1 n_{zz}^2 + K_3 n_{zz}^2
= (K_1 \cos^2 \theta + K_3 \sin^2 \theta) \theta_z^2.
\]
See [4, §3.1.2], [19, §2.2.1], [22, §3.2]. Here we denote $n_{x,z} = dn_x/dz$, $n_{z,z} = dn_z/dz$, and $	heta_z = d\theta/dz$. Thus the distortional free energy per unit area, $\tilde{F}_e := F_e/A$, as a function of the tilt angle $\theta$ is given by

$$\tilde{F}_e[\theta] = \frac{1}{2} \int_0^d \left( K_1 \cos^2 \theta + K_3 \sin^2 \theta \right) \theta_z^2 dz.$$ 

The appropriate contribution to the free-energy density associated with a static electric field arising from electrodes held at constant potential is

$$W_E = -\frac{1}{2} D \cdot E,$$

where $D$ is the displacement field and $E$ the electric field. This is discussed in a general context in [13, §4.7] and [15, §5, §10]; it is discussed in the particular context of liquid crystals in [2, §3.6.2, §3.6.3], [3, §10.1], and [23, §7.1]. Another perspective on this expression will be developed in §4.3. In a system such as ours (a transversely isotropic medium in the linear regime), it is usually assumed that

$$D = \epsilon(n) E, \quad \epsilon = \epsilon_0 \left[ \epsilon_\perp I + \epsilon_a (n \otimes n) \right], \quad \epsilon_a := \epsilon_\parallel - \epsilon_\perp,$$

with $\epsilon$ the dielectric tensor and $\epsilon_\perp$ and $\epsilon_\parallel$ the relative dielectric permittivities perpendicular to $n$ and parallel to $n$, giving

$$W_E = -\frac{1}{2} \epsilon_0 \left[ \epsilon_\perp E^2 + \epsilon_a (E \cdot n)^2 \right], \quad E = |E|.$$ 

The macroscopic modeling of electric fields in liquid crystals is discussed in [4, §3.3.1], [19, §2.3.1], and [22, §4.1]. We note that the electric field is in general nonhomogeneous [8] and that the linear relation between static $D$ and $E$ fields can be nonlocal in space, though such spatial dispersion is generally viewed as negligible in macroscopic models of pure dielectrics—see [13, §1.4] or [15, §103].

The relevant Maxwell equations for electrostatics (assuming no distribution of free charge in $\Omega$) are

$$\text{curl } E = 0, \quad \text{div } D = 0.$$ 

Tangential components of $E$ are continuous across a material interface, while the normal component of $D$ suffers a jump equal to the surface charge density $\sigma_i$ on the interface:

$$[E] = 0, \quad [D_\nu] = \sigma_i.$$ 

Both $D$ and $E$ vanish inside electrodes. The basic electrostatics that we require can be found in any of [13 Ch. I, Ch. 1], [15 Ch. I, Ch. II], [16 Chs. 2–6], or [20 Ch. III]. Using $\text{curl } E = 0$ and the interface conditions, we conclude that in our system

$$E = -U_z e_z, \quad U_z = dU/dz, \quad D_z(0+) = D_z(d-) = -\sigma,$$ 

with $U_z$ the electric potential.
where \( U = U(z) \) is the electric potential and \( \sigma \) is the (uniform) surface charge density on the upper electrode (\(-\sigma\) on the lower electrode). Given the polarity indicated in our circuit diagram in figure 1b, we have \( \sigma > 0 \). Thus \( W_E \) simplifies to
\[
W_E = -\frac{1}{2} \varepsilon_0 (\epsilon_\perp n^2_x + \epsilon_\parallel n^2_z) U^2_z.
\]

For equilibrium states of our model problem, then, the total free energy (per unit area) expressed as a functional of \( \theta \) and \( U \) is given by
\[
\tilde{F} [\theta, U] = \frac{1}{2} \int_0^d \left[ (K_1 \cos^2 \theta + K_3 \sin^2 \theta) \theta_z^2 - \varepsilon_0 (\epsilon_\perp \cos^2 \theta + \epsilon_\parallel \sin^2 \theta) U^2_z \right] dz.
\]

(6)

2.1 Coupled system

When viewed as a coupled system in this way, the equilibrium Euler-Lagrange equations that follow from \( \delta \theta \tilde{F} = 0 \) and \( \delta U \tilde{F} = 0 \) are given by
\[
\frac{d}{dz} \left[ (K_1 \cos^2 \theta + K_3 \sin^2 \theta) \theta_z \right] = \sin \theta \cos \theta \left[ (K_3 - K_1) \theta_z^2 - \varepsilon_0 \epsilon_\perp U^2_z \right],
\]

\[
\frac{d}{dz} \left[ (\epsilon_\perp \cos^2 \theta + \epsilon_\parallel \sin^2 \theta) U_z \right] = 0,
\]

(7a)

(7b)

with boundary conditions
\[
\theta(0) = \theta(d) = 0, \quad U(0) = -\Delta U/2, \quad U(d) = \Delta U/2.
\]

(7c)

Here \( \Delta U \) is the difference between the electric potential on the upper electrode and that on the lower electrode, and the director field and electric field in the cell depend only on this difference—an arbitrary constant added to \( U \) has no effect on solutions of \( (7) \) (one could just as well impose boundary conditions \( U(0) = 0, \quad U(d) = \Delta U \)). Equation \( (7b) \) corresponds to \( \text{div} \, D = 0 \) for our model cell and emerges in a natural way as a condition of stationarity of \( \tilde{F} [\theta, U] \).

The characterization of the stability properties of solutions of the coupled system \( (7) \) is a little nonstandard because of the “minimax” nature of the free energy \( \tilde{F} \) in \( (6) \). Locally stable solutions are locally minimizing with respect to \( \theta \) but maximizing with respect to \( U \); while globally stable solutions are globally minimizing with respect to \( \theta \), maximizing with respect to \( U \). Globally stable solutions can also be characterized as equilibrium solutions of least free energy. These topics are taken up in \( [8] \). From the point of view of dynamical stability, the picture is somewhat confusing, and a goal of this note is to try to understand this better.

2.2 Reduced system

Instead of viewing the system as a coupled system with two state variables, one can eliminate \( U \) and model the system in terms of \( \theta \) only. An integration of \( (7b) \) gives
\[
U_z = \Delta U \left[ \int_0^d \frac{dz}{\epsilon_\perp \cos^2 \theta + \epsilon_\parallel \sin^2 \theta} \right]^{-1} \frac{1}{\epsilon_\perp \cos^2 \theta + \epsilon_\parallel \sin^2 \theta}.
\]

(8)
which when substituted into (7a) produces

\[
\frac{d}{dz}
\left[
(K_1 \cos^2 \theta + K_3 \sin^2 \theta) \theta^2_z
\right] = \sin \theta \cos \theta \left\{ (K_3 - K_1) \theta^2_z
- \frac{\epsilon_0 \epsilon_a (|\Delta U|^2)}{2 (\epsilon_\perp \cos^2 \theta + \epsilon_\parallel \sin^2 \theta)^2}
\right\}.
\]

This same equation can be obtained from the first variation of the reduced free energy \( \tilde{F}_r \) that results when the expression for \( U_z \) above is substituted into (6):

\[
\tilde{F}_r[\theta] = \frac{1}{2} \int_0^d \left( K_1 \cos^2 \theta + K_3 \sin^2 \theta \right) \theta^2_z dz
- \frac{1}{2} \epsilon_0 (|\Delta U|^2) \left[ \int_0^d \frac{dz}{\epsilon_\perp \cos^2 \theta + \epsilon_\parallel \sin^2 \theta} \right]^{-1}.
\]

If the voltage of the battery is \( V \), then in equilibrium \( \Delta U = V \), and the above expression agrees with [19, (3.221)]. When the system is not in equilibrium, however, \( \Delta U \) need not be equal to \( V \), and this will be an issue in what follows.

The formulation in terms of the reduced free energy is natural and has been widely used. It was used by Deuling in [5], which is recounted in [19, §3.5]. It was used by Hardt, Kinderlehrer, and Lin in their analytical paper [12], and it was also employed by the author in [8]. The formulation has certain advantages in terms of stability assessment, in that locally stable states are local minimizers of \( \tilde{F}_r \) with respect to \( \theta \), and globally stable states are global minimizers (the second variation \( \delta^2 \tilde{F}_r \) being positive definite in both cases).

Using \( \tilde{F}_r \) is equivalent to minimizing the free energy \( \tilde{F} \) in the subject to the ODE constraint (7b). The approach amounts to viewing the electric field as slaved to the director field. A disadvantage of the reduced-free-energy formulation is that the equilibrium Euler-Lagrange equation (9) is nonlocal.

When the system is out of equilibrium and the director field is evolving in time \((n = n(z,t), \theta = \theta(z,t))\), then the capacitance of the liquid-crystal cell will be changing with time as well. In this case, the battery will need to move charge on or off the electrodes in order to re-establish the equilibrium potential difference \( \Delta U = V \). The associated currents in the electric circuit will suffer some energy loss, due to Joule heating, and we need a way to combine these effects with the dynamics and viscous dissipation in the liquid-crystal cell. We begin by reviewing the charge dynamics of a standard RC circuit.

### 3 RC circuits

The typical kind of experimental setup that we envision can be viewed as an RC circuit with the liquid-crystal cell forming a capacitor containing a complex time-varying dielectric, as depicted in figure [11]. The resistance \( R \) could come from the presence of an actual resistor, or it could just be thought of as a surrogate to account for the total resistance of all the elements in the circuit (wires, connectors, conduction layers in the cell, etc.). The equation governing charge dynamics in such a circuit follows from the Kirchhoff Voltage Law and the formulas for the potential drops across a resistor and a capacitor [16, §6.6, §7.8]:

\[
\Delta U_{\text{res}} = IR, \quad \Delta U_{\text{cap}} = \frac{Q}{C} \Rightarrow IR + \frac{Q}{C} = V.
\]
Here $Q(t)$ is the instantaneous total charge on the upper (positive) electrode, and $I = \frac{dQ}{dt}$ is the current. Appending an initial condition leads to the IVP

$$R \frac{dQ}{dt} + \frac{1}{C} Q = V, \quad Q(0) = Q_0,$$

the solution of which can be written

$$Q(t) = Q_\infty + (Q_0 - Q_\infty) \exp(-t/\tau), \quad Q_\infty := CV, \quad \tau := RC.$$

Thus the steady state of the circuit corresponds to

$$Q = CV, \quad \Delta U = V,$$

and the characteristic time scale for the dynamics is $\tau = RC$—from here on, we simply denote $\Delta U_{\text{cap}} = \Delta U$ (as we have used in the previous section).

The state of the circuit could just as well be characterized in terms of $\Delta U$ (instead of $Q$), in which case (11) would take the form

$$R \frac{d}{dt}(C\Delta U) + \Delta U = V, \quad \Delta U(0) = \Delta U_0.$$

As we shall see in what follows, $C$ depends on $n$ (which will be changing in time, leading to $C = C(t)$); so modeling the circuit in terms of $Q$ proves to be more convenient (at least for our model problem).

The potential energies of the capacitor and battery, relative to a value of zero at $Q = 0$, are given by

$$E_{\text{cap}} = \frac{1}{2} Q \Delta U, \quad E_{\text{bat}} = -QV.$$

The relation $Q = C\Delta U$ makes it possible to write these expressions in various equivalent forms, e.g., $E_{\text{cap}} = Q^2/2C$ or $E_{\text{cap}} = C(\Delta U)^2/2$. These potential energies correspond to the work done in a reversible process building up the charge on the capacitor electrodes in an incremental way. As the charge on the capacitor is being built up, the electric potential is changing there as well (according to the relation $Q = C\Delta U$), leading to the factor of $1/2$: the increment of work done in moving an increment of charge from a location of potential zero to a location of potential $\Delta U$ is $\delta W = \delta Q \Delta U$, giving

$$W_{\text{cap}} = \int_0^{Q_f} \Delta U \, dQ = \int_0^{Q_f} \frac{Q}{C} \, dQ = \frac{1}{C} \int_0^{Q_f} Q \, dQ = \frac{1}{2C} Q_f^2 = \frac{1}{2} Q_f \Delta U_f,$$

where $Q_f$ and $\Delta U_f$ are the final (fully charged) values of $Q$ and $\Delta U$. The battery, on the other hand, always maintains a constant potential of $V$; so

$$W_{\text{bat}} = \int_{Q_f}^0 V \, dQ = V \int_{Q_f}^0 dQ = -Q_f V.$$

A discussion of these textbook formulas can be found in [16, §6.6]. By convention, the accounting is done in terms of just the positive electrode, but it takes into account the
contribution of the negative electrode—in actuality, one has charge \( Q \) on the positive electrode at potential \( \Delta U / 2 \) and charge \(-Q\) on the negative electrode at potential \(-\Delta U / 2\). We conclude that the total potential energy at any instant, expressed in terms of \( Q \), is given by

\[
\mathcal{E} := \mathcal{E}_{\text{cap}} + \mathcal{E}_{\text{bat}} = \frac{1}{2C}Q^2 - QV.
\]

The discussion above assumes a constant capacitance \( C \). We will revisit this calculation later with \( C = C(Q) \).

We note that whether the system is in equilibrium or not, we always have equal and opposite total excess charge on the upper and lower electrode surfaces. This relates to conservation of charge and is a consequence of Gauss’s Law. In the full time-dependent Maxwell equations (as well as in Maxwell electrostatics), we always have \( \text{div} \, \mathbf{D} = 0 \) in the absence of any free-charge distribution in \( \Omega \) (which we have assumed to be the case throughout). From this follows

\[
0 = \int_{\Omega} \text{div} \, \mathbf{D} \, dV = \int_{\partial \Omega} \mathbf{D} \cdot \mathbf{n} \, dS = -\int_{\partial \Omega} \sigma T \, dS.
\]

In our system, \( \sigma T \) is supported on the top and bottom electrode surfaces; so the total charge on the top and bottom must sum to zero (\( Q \) on the top and \(-Q\) on the bottom, in our notation). We also note that we use interchangeably the terms “potential energy,” “electrostatic energy,” and “free energy”—all refer to the energy associated with reversible work processes.

Current flowing through a resistor leads to energy dissipation (by Joule heating) at a rate \( R I^2 \)—see [15, (21.6)] or [20, §1.8, (4)]. The Rayleigh dissipation function associated with this is

\[
\mathcal{R} = \frac{1}{2}RI^2 = \frac{1}{2}R \left( \frac{dQ}{dt} \right)^2.
\]

From a variational point of view, then, the circuit dynamics can be obtained from a dissipation principle:

\[
\partial \mathcal{E} / \partial Q + \partial \mathcal{R} / \partial Q = 0 \Rightarrow \frac{1}{C}Q - V + R \frac{dQ}{dt} = 0,
\]

in agreement with [11]. Here we follow the formalism of Lagrangian mechanics with frictional forces and potential energy only (no kinetic energy), denoted in that setting \( L = T - V = -V \) (with \( V = \mathcal{E} \) here)—see, for example, [18 §2.2.1], where a historical perspective and classical references can be found.

One can try to put some of this in context. The total energy dissipated in the dynamical process is given by

\[
\mathcal{D} = \int_0^\infty RI^2 \, dt = \frac{1}{2C} (Q_\infty^2 - Q_0^2),
\]

using (12), compared to the potential-energy changes of the capacitor and battery:

\[
\Delta \mathcal{E}_{\text{cap}} = \frac{1}{2C} (Q_\infty^2 - Q_0^2), \quad \Delta \mathcal{E}_{\text{bat}} = -(Q_\infty - Q_0)V = \frac{1}{C} (Q_0 - Q_\infty)Q_\infty.
\]
Thus we always have
\[ \Delta E_{\text{cap}} + \Delta E_{\text{bat}} + D = 0, \]
as we must. In the special case of charging the capacitor from zero \( Q_0 = 0 \), we have
\[ D = \Delta E_{\text{cap}} = \frac{1}{2} CV^2, \quad \Delta E_{\text{bat}} = -CV^2. \]

In this case, half the work done by the battery goes into the final electrostatic energy of the capacitor, while the other half is lost to dissipation. Similar phenomena (in which half of the work is lost to dissipation) occur in a number of other settings, including simple spring-mass-damper systems and linear elasticity [7].

At the other extreme, if the initial charge on the capacitor were just slightly out of equilibrium, \( Q_0 = (1 + \varepsilon)Q_\infty \), say, then one would obtain
\[ \Delta E_{\text{cap}} = -\varepsilon(1 + \varepsilon/2)CV^2, \quad \Delta E_{\text{bat}} = \varepsilon CV^2, \quad D = \varepsilon^2 CV^2 / 2. \]

In this case, both \( \Delta E_{\text{cap}} \) and \( \Delta E_{\text{bat}} \) are \( O(\varepsilon) \), but \( D = O(\varepsilon^2) \)—and the dissipation would essentially be negligible when \( |\varepsilon| \ll 1 \). While we always have
\[ 0 \leq D \leq |\Delta E_{\text{cap}}|, \]
we only have \( D = |\Delta E_{\text{cap}}| \) in the case \( Q_0 = 0 \) or in the trivial cases \( Q_0 = Q_\infty \) (no dynamics) or \( Q_\infty = 0 \) (no battery).

4 Total potential energy and dynamical system

There is a mutual influence between the director field in the cell and the state of the electric circuit: the director field determines the capacitance of the cell (which affects the circuit), while the state of the circuit (whether characterized by \( Q \) or by \( \Delta U \)) affects the electric field in the cell (and hence the director field). In order to put together a coupled set of equilibrium equations or dynamical equations, we require expressions for the total potential energy and for the dissipation of the full system. These, in turn, require certain “building blocks,” which we now derive.

4.1 Capacitance of the cell

Due to the simplicity of our model problem (fields depending on only one space variable, stratified nature of the dielectric), it is possible to express the capacitance of the cell in analytical form:
\[ C[n] = \epsilon_0 A \left[ \int_0^d \frac{dz}{\epsilon_n n_2^2 + \epsilon_\parallel n_2^2} \right]^{-1}. \]

This can be derived in various ways. Using the basic relation for a parallel-plate capacitor \( Q = C\Delta U \) (with \( Q \) the total charge on the positive electrode, \( C \) the capacitance, and \( \Delta U \) the potential difference), we have
\[ Q = \epsilon_0 A \left[ \int_0^d \frac{dz}{\epsilon_n n_2^2 + \epsilon_\parallel n_2^2} \right] \Delta U. \]
the potential difference between the electrodes, as before) and the relations in \([4]\) and \([5]\), we have

\[
D_z = \epsilon_{zz} E_z = -\sigma \Rightarrow U_z = -E_z = \frac{\sigma}{\epsilon_{zz}} \Rightarrow \Delta U = \int_0^d U_z \, dz = \sigma \int_0^d \frac{dz}{\epsilon_{zz}},
\]

which gives

\[
C = \frac{Q}{\Delta U} = \frac{\sigma A}{\sigma \int_0^d (1/\epsilon_{zz}) \, dz} = A \left[ \int_0^d \frac{dz}{\epsilon_{zz}} \right]^{-1} = \epsilon_0 A \left[ \int_0^d \frac{dz}{\epsilon_{\perp} n_x^2 + \epsilon_{\parallel} n_z^2} \right]^{-1}.
\]

In this situation, \(C\) is simply an integral functional of the director field. One also sees such expressions derived by approximating the stratified dielectric as a collection of thin capacitive elements in series \([6, \S 5.4.3.1]\). Note that if the material were isotropic with relative permittivity \(\epsilon_r\) (i.e., \(\epsilon_{\perp} = \epsilon_{\parallel} = \epsilon_r\)), then \((14)\) would simplify to \(C = \epsilon A/d\) with \(\epsilon = \epsilon_0 \epsilon_r\), which is the textbook expression for the capacitance of a parallel-plate capacitor \([16, \S 6.6]\).

In more general circumstances (such as a director field that is a function of more than one space variable), it is not possible to derive a formula such as the above: there is no explicit analytical expression for the capacitance of a cell with a two- or three-dimensional inhomogeneity of the dielectric. In such cases, one can characterize the capacitance in terms of the director field \(n\) in \(\Omega\) given either \(Q\) or \(\Delta U\), but to determine \(C\), one must solve an auxiliary problem from an appropriate formulation of Maxwell electrostatics, then determine \(\Delta U\) from this solution (if \(Q\) was given) or \(Q\) (if \(\Delta U\) was given), and finally compute the ratio \(C = Q/\Delta U\).

### 4.2 Potential energy of the cell

The textbook calculation of the electrostatic energy of a capacitor was recounted in \(\S 3\). When combined with the relation \(Q = C \Delta U\), it yielded several equivalent ways of writing this potential energy:

\[
\mathcal{E}_{\text{cap}} = \frac{1}{2} Q \Delta U = \frac{1}{2C} Q^2 = \frac{1}{2} C (\Delta U)^2. \tag{15}
\]

The calculation of \(\mathcal{E}_{\text{cap}}\) in \(\S 3\) depended on the assumption that the capacitance of the cell was constant. In our system, however, the capacitance changes with changes in the director field in the cell, and we must modify this calculation accordingly.

As before, we start from the fact that the increment of work \(\delta W\) done in moving an increment of charge \(\delta Q\) from one location to another location of potential difference \(\Delta U\) is \(\delta W = \delta Q \Delta U\), giving (as before)

\[
W_{\text{cap}} = \int_0^{Q_f} \Delta U \, dQ = \int_0^{Q_f} Q \frac{dQ}{C}.
\]

Now, however, \(C\) depends on \(Q\) (in a way that could be complicated and not easy to express)—as charge is added to the upper electrode (depleted from the lower electrode), the electric field in the cell will eventually become strong enough to distort the director.
field (and change the capacitance). An integration by parts provides a simple way to assess
the new situation:

\[ W_{\text{cap}} = \int_{0}^{Q_f} \frac{Q}{C(Q)} \, dQ = \int_{0}^{Q_f} \frac{1}{C(Q)} \, \left( \frac{Q^2}{2} \right) \, dQ = \frac{1}{2} \frac{Q_f^2}{C(Q_f)} + \frac{1}{2} \int_{0}^{Q_f} \frac{Q^2}{C(Q)^2} \, dQ \frac{dC}{dQ} \, dQ = \frac{1}{2} \frac{Q_f^2}{C(Q_f)} + \frac{1}{2} \int_{C(0)}^{C(Q_f)} (\Delta U)^2 \, dC. \]

The first term on the right-hand side above is one form of the electrostatic energy \( E_{\text{cap}} \) of a
 capacitor with a constant capacitance \( C = C(Q_f) \), as in (15). The second term above can be interpreted as follows.

The increment of work \( \delta W \) done in changing the capacitance by an incremental amount \( \delta C \) is
\( \delta W = \frac{1}{2} \frac{Q_f^2}{C(Q_f)} (\Delta U)^2 \), which can be seen from the alternate form of the potential energy
of the capacitor \( E_{\text{cap}} = \frac{1}{2} C(\Delta U)^2 \). Thus the integral term on the right-hand side above is the reversible work done in changing the capacitance of the cell from its initial value at \( Q = 0 \) to its final value at \( Q = Q_f \). In our system, the only way the capacitance can be changed is by distorting the director field in \( \Omega \), and the work function for that process is the
distortional elastic energy \( F_e \). Thus the integral in question gives the change in distortional
elastic energy from its value at \( Q = 0 \) to its value at \( Q = Q_f \):

\[ \frac{1}{2} \int_{C(0)}^{C(Q_f)} (\Delta U)^2 \, dC = F_e \bigg|_{Q=Q_f} - F_e \bigg|_{Q=0} = F_e \bigg|_{Q=Q_f}, \]

since \( F_e \bigg|_{Q=0} = 0 \) in our system. Under more general circumstances, one could have \( F_e \bigg|_{Q=0} \neq 0 \), but that term would just add a constant to the potential energy and could be ignored.

We see that the potential energy of the liquid-crystal cell in our system is given by

\[ W_{\text{cap}} = E_{\text{cap}} + F_e[n], \quad E_{\text{cap}} = \frac{1}{2} Q \Delta U = \frac{1}{2} C[n]^{-1} Q^2 = \frac{1}{2} C[n] (\Delta U)^2, \]

where \( n, Q, \) and \( \Delta U \) are the instantaneous values of these state variables. This expression
captures, in a clean and decoupled way, both the work done in moving charge and that
done by inducing change in the capacitance (by distorting the director field). We note that
we continue to use the notation \( E_{\text{cap}} \) for any of the equivalent formulas for the electrostatic
energy of a capacitor of constant capacitance \([15]\), with the understanding that the value
of \( C \) is always taken to be that associated with the current state of the director field:
\( C = C[n] \).

4.3 Potential energy of the system and coupled equilibrium equations

The total potential energy of the system \( G \) is thus given by

\[ G = F_e + E_{\text{cap}} + E_{\text{bat}} = F_e + \frac{1}{2} Q \Delta U - QV. \]
for $G$ can be related to more familiar forms by noting that for static electric fields, $E_{\text{cap}}$ can be expressed in terms of field intensities inside the cell:

$$\frac{1}{2} Q\Delta U = \frac{1}{2} \int_{\Omega} (D \cdot E) \, dV,$$

(17)

where $D$ and $E$ are the fields associated with the electrostatic problem $\text{div} \, D = 0$ in $\Omega$ with a potential difference $\Delta U$ between the electrodes. This can be established as follows. Using the relations $D \cdot \nu = -\sigma_f$ (with $\nu$ the outward normal from $\Omega$), $\text{div} \, D = 0$, and $E = -\nabla U$, we obtain the following relation for a general surface charge density $\sigma_f$ and electric potential $U$:

$$\int_{\partial \Omega} \sigma_f U \, dS = -\int_{\partial \Omega} (UD) \cdot \nu \, dS = -\int_{\Omega} \text{div}(UD) \, dV$$

$$= -\int_{\Omega} (U \text{div} \, D + \nabla U \cdot D) \, dV = \int_{\Omega} (D \cdot E) \, dV.$$

See, for example, [16, §6.3] or [20, §2.8]. In our system, the surface charge density is supported on the upper and lower boundary electrodes, and the electric potential $U$ is constant on each electrode ($-\Delta U/2$ on the lower, $\Delta U/2$ on the upper), giving

$$\int_{\partial \Omega} \sigma_f U \, dS = \int_{\Gamma_1} \sigma_f U \, dS + \int_{\Gamma_2} \sigma_f U \, dS = -\frac{\Delta U}{2} \int_{\Gamma_1} \sigma_f \, dS + \frac{\Delta U}{2} \int_{\Gamma_2} \sigma_f \, dS$$

$$= -\frac{\Delta U}{2} (-Q) + \frac{\Delta U}{2} Q = Q\Delta U.$$

Here $\Gamma_1$ and $\Gamma_2$ are the lower and upper boundary electrode interfaces. Combining these two calculations establishes the validity of (17). Note that this argument does not require $\sigma_f$ to be constant on $\Gamma_1$ or $\Gamma_2$.

Concerning these equivalent formulas for electrostatic energy

$$\frac{1}{2} \int_{\partial \Omega} \sigma_f U \, dS = \frac{1}{2} \int_{\Omega} (D \cdot E) \, dV,$$

the left-hand side is in fact the more primitive expression (how electrostatic energy associated with surface charge distributions is often first derived in electromagnetics textbooks)—see, for example, [16, §6.2] or [20, §2.7]. We note that when there is no current flowing in the circuit, then $\Delta U = V$, and the combination $E_{\text{cap}} + E_{\text{bat}}$ satisfies

$$E_{\text{cap}} + E_{\text{bat}} = \frac{1}{2} QV - QV = -\frac{1}{2} QV = -\frac{1}{2} \int_{\Omega} (D \cdot E) \, dV,$$

(18)

which is the appropriate contribution to the free energy to be used in modeling liquid crystal equilibrium states in a setting such as ours. We emphasize that in order for (18) to be valid, one requires equilibrium conditions in the electrical circuit ($I = 0, \Delta U = V$) and also equilibrium of the electric field in the cell ($\text{curl} \, E = 0, E = -\nabla U$)—with time-varying electric fields, the time-dependent Maxwell equations have $\text{curl} \, E \neq 0$, in general, and $E$ cannot be expressed as the gradient of a scalar potential.
The expression for $G$ in \((16)\) can be written in different forms, depending upon the choice of state variable for the circuit:

\[
G[n, \Delta U] = \mathcal{F}_e[n] + C[n] \left[ \frac{1}{2} (\Delta U)^2 - V \Delta U \right]
\]

or

\[
G[n, Q] = \mathcal{F}_e[n] + \frac{1}{2} C[n]^{-1} Q^2 - VQ.
\]

Here $n$ is the current state of the director field in $\Omega$, $\mathcal{F}_e[n]$ is the distortional elastic energy of that state (as in \((2)\)), and $C[n]$ is the capacitance of the cell in that state (given by \((14)\) for our model problem). The above expressions apply more generally than just to our model problem; they are valid, for example, even if the fields in the cell depend on more than one space variable (though in that case, one would not have an explicit formula for $C[n]$, in general).

Stable equilibrium states of the system correspond to minimizers of the total potential energy $G$ with respect to $(n, \Delta U)$ or $(n, Q)$, depending on the choice of state variables. The capacitance is positive; so

\[
\text{min } G \Rightarrow \Delta U = V, \ Q = CV,
\]

and the following minimization problem for $n$ results:

\[
\text{min}_n \left\{ \mathcal{F}_e[n] - \frac{1}{2} C[n] V^2 \right\}.
\]

Using \((17)\) and the equilibrium condition $Q = C[n] V$, the objective functional above can be written

\[
\mathcal{F}_e[n] - \frac{1}{2} C[n] V^2 = \mathcal{F}_e[n] - \frac{1}{2} \int_\Omega (D \cdot E) \, dV.
\]

Here the terms $D$ and $E$ in the last integral correspond to the solution of the electrostatics problem in $\Omega$ with the dielectric tensor associated with the current director field, $\epsilon = \epsilon(n)$, and with a potential difference of $V$ across the cell. The minimization with respect to $n$ is subject to the pointwise constraint $|n| = 1$ and appropriate boundary conditions. The functional $\mathcal{F}_e - \frac{1}{2} \int_\Omega (D \cdot E) \, dV$ is the correct form of the free energy for equilibrium states of $n$ in an electric field, as in \((1)\) (with the identification $D = \epsilon(n) E$, $E = -\nabla U$).

All of these expressions can be put in explicit forms for our model problem, for which it is convenient to use the formulation in terms of $Q$. The state variables are $n = n(z, t)$ (the director field in the cell) and $\sigma = \sigma(t)$ (the charge density on the upper electrode). Scaling our energies and capacitance by the cross-sectional area of the cell,

\[
\tilde{G} := \frac{G}{A}, \hspace{1em} \tilde{\mathcal{F}}_e := \frac{\mathcal{F}_e}{A}, \hspace{1em} \tilde{C} := \frac{C}{A},
\]

and using $Q = \sigma A$, we obtain

\[
\tilde{G}[n, \sigma] = \tilde{\mathcal{F}}_e[n] + \frac{1}{2} \tilde{C}[n]^{-1} \sigma^2 - \sigma V
\]

\[
= \frac{1}{2} \int_0^d \left( K_1 n_z^2 + K_3 n_z^2 \right) \, dz + \frac{1}{2} \frac{\sigma^2}{\epsilon_0} \int_0^d \frac{dz}{\epsilon_\parallel n_z^2 + \epsilon_\parallel n_z^2} - \sigma V.
\]
Here we have used (2), (3), and (14) to provide the expressions for $F[n]$ and $C[n]$. We shall work with this mostly in terms of the tilt-angle representation $n = \cos \theta e_x + \sin \theta e_z$:

$$\tilde{G}[\theta, \sigma] = \frac{1}{2} \int_0^d \left( K_1 \cos^2 \theta + K_3 \sin^2 \theta \right) \theta_z^2 \, dz + \frac{1}{2} \frac{\sigma^2}{\varepsilon_0} \int_0^d \frac{dz}{\varepsilon_{\perp} \cos^2 \theta + \varepsilon_{\parallel} \sin^2 \theta} - \sigma V. \quad (20)$$

The associated coupled equilibrium equations from $\delta \tilde{G} = 0$ and $\partial \tilde{G}/\partial \sigma = 0$ are

$$\frac{d}{dz} \left[ (K_1 \cos^2 \theta + K_3 \sin^2 \theta) \theta_z \right] = \sin \theta \cos \theta \left[ (K_3 - K_1) \theta_z^2 - \frac{\sigma^2}{\varepsilon_0} \frac{1}{(\varepsilon_{\perp} \cos^2 \theta + \varepsilon_{\parallel} \sin^2 \theta)^2} \right],$$

$$\frac{\sigma}{\varepsilon_0} \int_0^d \frac{dz}{\varepsilon_{\perp} \cos^2 \theta + \varepsilon_{\parallel} \sin^2 \theta} = V.$$

The latter equation is equivalent to $Q = CV$, which is the correct equilibrium condition for the charge. Substituting the equilibrium value for $\sigma$ above into (20) and into the equilibrium ODE for $\theta$ above correctly gives the reduced free energy (10) and equilibrium equation (9), in agreement with [19, (3.221), (3.226)].

4.4 Dissipation and dynamics

We wish to use a dissipation principle to obtain a dynamical system involving the coupled state variables $n$ and $\sigma$. The simplest expression for dissipation associated with the dynamics of the director field is usually given in terms of the single rotational viscosity parameter $\gamma_1$ via the Rayleigh function

$$\frac{1}{2} \gamma_1 \int_{\Omega} \left| \frac{\partial n}{\partial t} \right|^2 \, dV = \frac{1}{2} \gamma_1 A \int_0^d \left( \frac{\partial \theta}{\partial t} \right)^2 \, dz =: \tilde{R}_\theta.$$

Per unit area, then, we have

$$\tilde{R}_\theta := \frac{1}{A} \tilde{R}_\theta = \frac{1}{2} \gamma_1 \int_0^d \left( \frac{\partial \theta}{\partial t} \right)^2 \, dz.$$

We have already seen in (13) that the Rayleigh dissipation function for the electric circuit is

$$\frac{1}{2} R \left( \frac{dQ}{dt} \right)^2 = \frac{1}{2} RA^2 \left( \frac{d\sigma}{dt} \right)^2 =: \tilde{R}_\sigma,$$

which leads to

$$\tilde{R}_\sigma := \frac{1}{A} \tilde{R}_\sigma = \frac{1}{2} RA \left( \frac{d\sigma}{dt} \right)^2.$$

Combining these gives

$$\tilde{\mathcal{R}} := \tilde{R}_\theta + \tilde{R}_\sigma = \frac{1}{2} \gamma_1 \int_0^d \left( \frac{\partial \theta}{\partial t} \right)^2 \, dz + \frac{1}{2} RA \left( \frac{d\sigma}{dt} \right)^2,$$

which is the form we shall adopt for our combined dissipation function.
The total potential energy \( \partial \tilde{G} / \partial \sigma \) and Rayleigh function \( \partial \tilde{R} / \partial \dot{\sigma} \) produce the correct circuit dynamics:

\[
\frac{\partial \tilde{G}}{\partial \sigma} + \frac{\partial \tilde{R}}{\partial \dot{\sigma}} = 0 \Rightarrow \frac{\sigma}{\epsilon_0} \int_0^d \frac{dz}{\epsilon_\perp \cos^2 \theta + \epsilon_\parallel \sin^2 \theta} - V + RA \frac{d\sigma}{dt} = 0 \Rightarrow R \frac{dQ}{dt} + \frac{1}{C} Q = V,
\]

using \( \epsilon_0 \) and \( Q = \sigma A \) — this agrees with \( \epsilon_0 \). The dynamics for the director angle results from the analogous expression for \( \theta \):

\[
\delta \theta \tilde{G} + \delta \dot{\theta} \tilde{R} = 0 \Rightarrow \frac{\partial W}{\partial \theta} - \frac{\partial}{\partial z} \left( \frac{\partial W}{\partial \theta} \right) + \frac{\gamma_1}{t} \frac{\partial \theta}{\partial t} = 0,
\]

with \( W \) the free-energy density that results from combining the integrated terms in \( \tilde{G} \).

In expanded form, the PDE for \( \theta \) is given by

\[
\gamma_1 \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left( (K_1 \cos^2 \theta + K_3 \sin^2 \theta) \frac{\partial \theta}{\partial z} \right) - \sin \theta \cos \theta \left( (K_3 - K_1) \left( \frac{\partial \theta}{\partial z} \right)^2 - \epsilon_a \frac{\sigma^2}{\epsilon_0 (\epsilon_\perp \cos^2 \theta + \epsilon_\parallel \sin^2 \theta)^2} \right),
\]

(22a)

Our dynamical system, then, consists of the PDE (22a) above for \( \theta \), supplemented by auxiliary conditions

\[
\theta(0, t) = \theta(d, t) = 0, \quad \theta(z, 0) = \theta_0(z),
\]

(22b)

and the ODE IVP for \( \sigma \)

\[
RA \frac{d\sigma}{dt} + \frac{\sigma}{\epsilon_0} \int_0^d \frac{dz}{\epsilon_\perp \cos^2 \theta + \epsilon_\parallel \sin^2 \theta} = V, \quad \sigma(0) = \sigma_0,
\]

(22c)

with the initial states \( \theta_0 \) and \( \sigma_0 \) prescribed. The variational approach used here to obtain the director dynamics equation (22a) is similar to that given in \[19, \S 4.3\] — compare (22a) with \[19, (4.152)\]. See also \[19, \S 5.9\], where the same ideas are used to model the dynamics of certain Fréedericksz transitions.

Some of the terms above can be related to more familiar expressions. The term involving \( \sigma^2 \) in (22a) corresponds to the “dielectric torque” \( D \times E \), the couple per unit volume exerted by the electric field on the director field. In our system, as in \[14\] and \( (5) \), we have

\[
E = E_{e \perp}, \quad D = \epsilon(n) E = \epsilon_0 E [\epsilon_a n_x n_x e_x + (\epsilon_\perp n_x^2 + \epsilon_\parallel n_z^2) e_z],
\]

In terms of \( \theta \), then,

\[
D \times E = -\epsilon_0 \epsilon_a E^2 \sin \theta \cos \theta e_y.
\]

The connection between \( E^2 \) and \( \sigma^2 \) follows from

\[
\sigma = -D_z \Rightarrow \sigma^2 = \epsilon_a^2 E^2 (\epsilon_\perp \cos^2 \theta + \epsilon_\parallel \sin^2 \theta)^2,
\]

which gives

\[
D \times E = -\epsilon_a \frac{\sigma^2}{\epsilon_0 (\epsilon_\perp \cos^2 \theta + \epsilon_\parallel \sin^2 \theta)^2} \sin \theta \cos \theta e_y,
\]

(22a)
as in (22a). Also, using (14) we have
\[
C[\theta]^{-1} = \frac{1}{\epsilon_0 A} \int_0^d \frac{dz}{\epsilon_\perp \cos^2 \theta + \epsilon_\parallel \sin^2 \theta},
\]
and (22c) can be written
\[
RA \frac{d\sigma}{dt} + C[\theta]^{-1} A \sigma = V \quad \text{or} \quad R \frac{dQ}{dt} + C[\theta]^{-1} Q = V,
\]
as in (11).

As we have already noted (and as we shall see in §4.6), the time scale for (22c) is often faster than that for (22a). If one were to choose to model the charge distribution as adjusting instantaneously to changes in the director field, then one would have \( d\sigma/dt = 0 \) in (22c), and that equation would collapse to the equilibrium condition for \( \sigma \) in the previous section. Substituting the equilibrium value for \( \sigma \) into (22a) would give the director-dynamics equation for the reduced free energy \( \tilde{F} \) in (10) (with \( \Delta U = V \)), that is, the dynamical version of (9) (again with \( \Delta U = V \)).

4.5 Time-varying \( D \) versus \( E \)

With an electric field that varies in space and in time \( (E = E(x,t)) \), the linear relationship between \( D \) and \( E \) is in general nonlocal in space and in time; however, for macroscopic models of pure dielectrics, nonlocality in space can generally be ignored [13, §I.4], [15, §77, §78, §103]. Nonlocality in time can be an issue in some circumstances, such as fast-switching experiments with electric fields from electric pulses of large voltage and short duration [11].

If the dielectric properties of the medium remain constant, spatial dispersion is ignored, and the electric field is time harmonic, then the induced polarization will be time harmonic with the same frequency and hence so will \( D \) (via \( D = \epsilon_0 E + P \)):

\[
E(x,t) = e^{-i\omega_0 t} E_0(x) \quad \Rightarrow \quad D(x,t) = e^{-i\omega_0 t} \epsilon(x,\omega_0) E_0(x).
\]

See [13 §I.4], [15 §77]. This includes the special case of a static electric field \( (\omega_0 = 0) \): \( D(x) = \epsilon(x) E(x) \).

The relationship between \( D \) and \( E \) in the time-harmonic case is frequency dependent, however \( (\epsilon = \epsilon(x,\omega)) \), and so for a general time-varying electric field (again in a medium of constant dielectric properties and no spatial dispersion), one has

\[
D(x,t) = \epsilon_0 E(x,t) + \epsilon_0 \int_{-\infty}^t \alpha(x,t-t')E(x,t') \, dt',
\]
as written in [11]. The tensor field \( \alpha \) comes from the inverse Fourier transform of the dispersion relation, that is,

\[
\epsilon(x,\omega) = \epsilon_0 \left[ I + \int_{-\infty}^{\infty} e^{i\omega t} \alpha(x,t) \, dt \right].
\]
An illustrative example (for a homogeneous, isotropic medium) is given in [13, §7.10], where a “one-resonance dispersion model” is employed (a complex rational function of $\omega$). The poles of the dispersion model are in the lower half of the complex $\omega$ plane, which gives rise to a one-sided inverse Fourier transform and an appropriately causal relationship of the form (23). From a physical point of view, at high frequencies, changes in the induced polarization can lag changes in the electric field. An electric pulse resolves into Fourier modes of arbitrarily high frequency, and because of this, these nonlocal-in-time effects (“dielectric relaxation”) can become important. In [11] and [17], the term “Dielectric Memory Effects” is used to describe them.

The dynamics of liquid-crystal systems induced by time-varying electric fields is even more complicated, since in that case, the dielectric properties of the medium are changing in time as well, and the convolution representation (23) is no longer valid. A research program described in the review article [17] (which contains references to earlier works) addressed this issue and developed a generalization of (23) to the case of a time-varying director field $\mathbf{n} = \mathbf{n}(\mathbf{x}, t)$. The theory was used to model successfully the experiments with fast-switching (pulse-driven) dynamics of [21] and others.

These issues are beyond the scope of our investigation here. Our assessment is that the local relationship $\mathbf{D} = \epsilon \mathbf{E}$ is valid in static equilibrium and more generally if $\mathbf{E}$ is time harmonic and the dielectric properties of the medium are constant. The relationship $\mathbf{D} = \epsilon \mathbf{E}$ is a good approximation if $\mathbf{E}$ contains only low-frequency content and the director dynamics are relatively slow. For our purposes here, we accept and adopt the local relationship $\mathbf{D} = \epsilon \mathbf{E}$ and acknowledge the limitations and shortcomings of that in some settings.

4.6 Time scales

The dynamic processes associated with a system such as the one under consideration here exhibit several different time scales, including those for director dynamics, circuit dynamics, and the evolution of the electric field in the cell. The time scales for the changes in the circuit and for the dynamics of the director field can be gleaned from rescalings of (22c) and (22a). First, it is convenient to relate the integral expression in (22c) to the capacitance (14) as follows:

$$C[\theta] = \epsilon_0 A \left[ \int_0^d \frac{dz}{\epsilon_\perp \cos^2 \theta + \epsilon_\parallel \sin^2 \theta} \right]^{-1} = \epsilon_0 A \frac{d}{d} \epsilon_t[\theta],$$

where $\epsilon_t[\theta]$ is the effective relative dielectric constant of the cell, given by

$$\epsilon_t[\theta]^{-1} = \frac{1}{d} \int_0^d \frac{dz}{\epsilon_\perp \cos^2 \theta + \epsilon_\parallel \sin^2 \theta}.$$

This quantity is dimensionless, $O(1)$, and satisfies

$$\epsilon_\perp \leq \epsilon_t[\theta] \leq \epsilon_\parallel,$$

since $\epsilon_\perp < \epsilon_\parallel$ for our system. In terms of it, (22c) can be written

$$\tau_\sigma \frac{d\bar{\sigma}}{dt} + \epsilon_t[\theta]^{-1} \bar{\sigma} = 1, \quad \tau_\sigma := R \frac{\epsilon_0 A}{d}, \quad \bar{\sigma} := \frac{\sigma}{\epsilon_0 V/d}. \quad (24a)$$
Note that $\epsilon_0 A/d$ would be the capacitance of the cell and $\epsilon_0 V/d$ would be the surface charge density on the upper electrode if there were a vacuum between the electrodes. Note also that in steady state, we have $d\sigma/dt = 0$ and $\sigma = \epsilon_t[\theta]$.

For a fairly typical experimental setup, the “RC load” $\tau_\sigma$ is generally in the sub-microsecond range. For example, with $R = 100 \Omega$, $\epsilon_0 = 8.854 \times 10^{-12} \text{F/m}$, $A = 10 \text{cm}^2$, and $d = 5 \mu\text{m}$, we obtain $\tau_\sigma \approx 1.77 \times 10^{-7} \text{s}$. In [14], $\tau_\sigma$ is estimated to be $2 \mu\text{s}$ and is a limiting factor in the experiment presented there. In the fast-switching experiments discussed in [11] and [21], measures are taken to minimize $\tau_\sigma$ (including the use of gold connectors to minimize resistance and cells of small area to minimize capacitance), and values for $\tau_\sigma$ in the nanosecond range are reported.

If one scales $z$ by the cell gap ($\bar{z} = z/d$), then (22a) can be put in the form

$$\frac{\partial \theta}{\partial t} = \frac{1}{\tau_K} \left\{ \frac{\partial}{\partial z} \left[ (K_1 \cos^2 \theta + K_3 \sin^2 \theta) \frac{\partial \theta}{\partial z} \right] \right\} - \sin \theta \cos \theta (K_3 - K_1) \left( \frac{\partial \theta}{\partial z} \right)^2$$

$$+ \frac{1}{\tau_V} \sigma^2 \frac{\sin \theta \cos \theta}{(\epsilon_1 \cos^2 \theta + \epsilon_3 \sin^2 \theta)^2},$$

(24b)

where

$$\tau_K := \frac{\gamma_1 d^2}{K}, \quad \tau_V := \frac{\gamma_1 d^2}{\epsilon_0 \epsilon_a V^2}, \quad K_1 := \frac{K_1}{K}, \quad K_3 := \frac{K_3}{K},$$

(24c)

with $K$ a representative value for $K_1$ and $K_3$. This exposes two times scales associated with director reorientation: $\tau_K$ and $\tau_V$. These correspond to “switch off” and “switch on” times, which are usually written

$$\tau_{off} = \frac{\gamma_1 d^2}{K \pi^2}, \quad \tau_{on} = \frac{\gamma_1}{\epsilon_0 \epsilon_a E^2}.$$

See [19] §5.9.

The switch-off time $\tau_{off}$ is the time scale for the slowest decaying mode of $\gamma_1 \theta_t = K \theta_{zz}$, $\theta(0) = \theta(d) = 0$. It gives the time it takes for a distorted director field to relax back to its ground state under the influence of only distortional elastic forces. This is a relatively slow process, usually estimated to be in the range of 10s of milliseconds for typical cells and materials (e.g., with $\gamma_1 = 0.1 \text{Pa s}$, $d = 5 \mu\text{m}$, and $K = 10 \mu\text{N}$, we obtain $\tau_{off} = 2.53 \times 10^{-2} \text{s}$).

The switch-on time $\tau_{on} = \tau_V$ (with $E = V/d$) corresponds to the time it takes to align the director field with an applied electric field. It can be made quite small by using large voltages. For example, with $\gamma_1 = 0.1 \text{Pa s}$, $d = 5 \mu\text{m}$, $\epsilon_0 = 8.854 \times 10^{-12} \text{F/m}$, $\epsilon_a = 10$, and $V = 100 \text{volts}$, we have $\tau_V \approx 2.82 \times 10^{-6} \text{s}$. For small voltages near the Fréedericksz threshold, on the other hand (e.g., with $V = 1 \text{volt}$), we have $\tau_V \approx 2.82 \times 10^{-2} \text{s}$. In the fast-switching experiments in [4, 11, 21], using cells of narrow gaps and electrical pulses of 100s of volts, $\tau_V$’s of the order of 10s of nanoseconds are reported.

By comparison, the evolution of the electric field in the cell is governed by the time-dependent Maxwell equations, and the time scale associated with this type of wave equation (which we denote $\tau_E$) corresponds to the width of the cell gap divided by the speed of light in the medium. For a cell gap $d = 10 \mu\text{m}$ with relative dielectric permittivity $\epsilon_t = 10$ and relative magnetic permeability $\mu_t = 1$, we obtain $\tau_E \approx 1.05 \times 10^{-13} \text{s}$, which is four orders
of magnitude faster than the smallest $\tau_\sigma$'s and $\tau_V$'s we have found in published results on experiments on fast switching of liquid crystal cells. This justifies treating the electric field as adjusting instantaneously to any changes in the circuit and cell.

Thus, for the kinds of experimental systems that we have in mind, we consider time scales in the following ranges:

$$10^{-9} \text{s} \lesssim \tau_\sigma \lesssim 10^{-6} \text{s}, \quad 10^{-8} \text{s} \lesssim \tau_K \lesssim 10^{-2} \text{s}, \quad 10^{-8} \text{s} \lesssim \tau_V \lesssim 10^{-2} \text{s}, \quad \tau_E \approx 10^{-13} \text{s}.$$ 

In the numerical examples discussed in the next section, we have taken $\tau_\sigma = 10^{-6} \text{s}$, $\tau_K = 10^{-2} \text{s}$, and $\tau_V = 10^{-7} \text{s}$, for purposes of illustration, with the electric field taken to adjust instantaneously ($\tau_E = 0$, in essence, as we have assumed throughout).

5 Numerical illustration

We illustrate the coupled dynamics of (22) by the numerical modeling of a simple “switch on” experiment. For simplicity, we assume equal elastic constants: $K_1 = K_3 = K$. Starting from the partially scaled system (24), we express times in units of $\tau_\sigma$ to obtain

\begin{align*}
\frac{d\bar{\sigma}}{dt} + \epsilon_i[\theta]^{-1}\bar{\sigma} &= 1, \quad \epsilon_i[\theta]^{-1} = \int_0^1 \frac{d\bar{\varepsilon}}{\epsilon_\perp \cos^2 \theta + \epsilon_\parallel \sin^2 \theta}, \quad (25a) \\
\frac{\partial \theta}{\partial \bar{\tau}} &= \frac{1}{\bar{\tau}_K} \frac{\partial^2 \theta}{\partial \bar{\varepsilon}^2} + \frac{1}{\bar{\tau}_V} \frac{\partial \sigma^2}{\bar{\tau}_V} \frac{\sin \theta \cos \theta}{(\epsilon_\perp \cos^2 \theta + \epsilon_\parallel \sin^2 \theta)^2}, \quad 0 < \bar{\varepsilon} < 1, \quad (25b)
\end{align*}

where

$$\bar{\tau}_i := \frac{t}{\tau_\sigma}, \quad \bar{\tau}_K := \frac{\tau_K}{\tau_\sigma}, \quad \bar{\tau}_V := \frac{\tau_V}{\tau_\sigma}.$$ 

We add a small pretilt to the boundary conditions on $\theta$, in order to bias the director to rotate counter clockwise when the electric field is switched on, and we take the initial state of the director field to be parallel to this. There is assumed to be no excess charge on the electrodes when the circuit is closed at time $\bar{\tau} = 0$. The boundary and initial conditions are thus given by

$$\theta(0, \bar{\tau}) = \theta(1, \bar{\tau}) = 0.1, \quad \theta(\bar{\varepsilon}, 0) = 0.1, \quad \bar{\sigma}(0) = 0. \quad (25c)$$

For the relative dielectric permittivities, we use $\epsilon_\perp = 5$ and $\epsilon_\parallel = 15$, which are comparable to the values for the typical liquid crystal 5CB—see [19, Appendix D, Table D.3]. Based upon the discussion of time scales in the previous section, we choose the following values for our numerical experiment:

$$\tau_K = 10^{-2} \text{s}, \quad \tau_\sigma = 10^{-6} \text{s}, \quad \tau_V = 10^{-7} \text{s}, \quad 10^{-6} \text{s}, \quad 10^{-5} \text{s},$$

giving

$$\bar{\tau}_K = 10^4, \quad \bar{\tau}_V = 10^{-1}, \quad 10^0, \quad 10^1.$$ 

The three values of $\bar{\tau}_V$ cover the situations when the director switching dynamics are faster than, equal to, and slower than the circuit dynamics.
Standard finite differences were employed to discretize our model (25): explicit Euler for (25a), Forward Time Centered Space (FTCS) for (25b). The same time step was used for both equations (Δt = 0.1, 10 times steps per unit τσ), with a spatial grid of 128 uniform cells in z. A Composite Trapezoid Rule (on the same spatial grid) was used to approximate the integral in the functional εr[θ] in (25a). For each of the values τv = 10−1, 100, and 101, σ is plotted against t, along with “time snapshots” of θ versus z for every 16th time step. In all three cases, the same number of time steps per snapshot (16) and the same number of total time steps (1024) were used, in order to facilitate comparison. The results are presented in figure 2.

The results are as one would anticipate. The case τv = 10−1 corresponds to a high voltage and fast switching: the director quickly saturates (after 5–6 snapshots), and the charge density behaves accordingly (σ ≈ ε∥(1−e−t)). We note that in the steady state limit t → ∞, we have σ → ε∥[θ∞] ≈ ε∥, since θ∞ ≈ π/2 (except for boundary layers near z = 0 and z = 1). The case τv = 100 corresponds to a moderate voltage and switching (τv = τσ): θ saturates after 15–16 snapshots, and one starts to see an inflection in σ. The last case, τv = 101, is associated with a low voltage and slow switching: it takes 50–60 snapshots for the director to align with the electric field, and one sees a pronounced inflection in σ versus t. This is because the time scale for the σ dynamics is approximately Reε⊥A/d in the early stages (when θ ≈ 0 and ε∥[θ] ≈ ε∥), but the time scale is approximately Reε∥A/d in the later stages (when θ ≈ π/2 and ε∥[θ] ≈ ε∥). Since ε⊥ = 5 and ε∥ = 15, these time scales differ by a factor of three, and this leads to the change in the rate of approach of σ to its limiting value. We emphasize that this is merely an illustration of the coupled dynamics that emerge from our simple model; in order to model carefully the dynamics in an actual fast-switching experiment, for example, one would need to take into account other influences, such as “dielectric relaxation” [11, 17].

6 Conclusions

We have modeled a nematic-liquid-crystal cell subject to an electric field created by electrodes held at constant potential as a variable capacitor in an RC circuit. The general model couples the state of the liquid-crystal director field n in the cell with the state of the electric circuit, characterized in terms of either the total charge on the upper electrode, Q, or the potential difference between the electrodes, ΔU. A dynamical system was derived for an example in the splay-Fréedericksz geometry, subject to several simplifying assumptions: no fluid flow in the cell, an electric field that adjusts instantaneously to changes in n, fields in the cell that are functions of one space variable only, and a single rotational viscosity for energy dissipation associated with ∂n/∂t. The dynamical system, given in (25), involves a PDE for director dynamics (n = n(z, t)) coupled to an ODE for charge dynamics (σ = σ(t), where σ is the density of free charge on the surface of the upper electrode). We have produced estimates for the time scales of the various dynamic processes and have provided numerical examples illustrating the coupled dynamics for three different cases relating the time scale for director dynamics to that of the circuit dynamics. We have made an effort to show consistency with established results, where possible.
Figure 2: Coupled dynamics \[25\]. Figures 2a, 2c, 2e: electrode charge density versus time \((\bar{\sigma} = \sigma/(\varepsilon_0V/d), \bar{t} = t/\tau_\sigma)\). Figures 2b, 2d, 2f: time snapshots of director tilt angle $\theta$ versus position \((\bar{z} = z/d, 16$ time steps per snapshot, time step $\Delta \bar{t} = 0.1)\). Parameters: $\varepsilon_\perp = 5$, $\varepsilon_\parallel = 15$, $\bar{\tau}_K = \tau_K/\tau_\sigma = 10^4$, $\bar{\tau}_V = \tau_V/\tau_\sigma = 10^{-1}$ (figures 2a, 2b), $10^0$ (figures 2c, 2d), $10^1$ (figures 2e, 2f).
The original motivation for this exercise was to understand better the dynamical characterization of local stability of equilibrium states of such systems, which can be characterized as stationary points of a free-energy functional of the form (1):

$$F[n, U] = \int_{\Omega} \left[ W_e(n, \nabla n) - \frac{1}{2} \epsilon(n) \nabla U \cdot \nabla U \right] dV.$$  

Here $\epsilon$ is the (positive definite) dielectric tensor and $U$ is the electric potential (related to the electric field $E$ via $E = -\nabla U$). The minimax nature of the critical points of $F$ is at odds with the expected picture of an out-of-equilibrium pair $(n, U)$ relaxing to a locally stable state by minimizing free energy. This confusion, as we have seen from our analysis, stems from the fact that the free-energy functional above presumes either a static electric field or an electric field that adjusts instantaneously to changes in $n$.

The more primitive expression for the potential energy of the system is $G$ as in (16):

$$G = F_e + E_{\text{cap}} + E_{\text{bat}} = F_e + \frac{1}{2} Q \Delta U - QV.$$  

Here $F_e$ is the distortional elasticity, as in (2) and (3), and $V$ is the voltage of the battery. The combination $F_e + E_{\text{cap}}$ gives the potential energy of the cell (associated with the work done in distorting the director field plus work done in moving charge on/off the electrodes); while $E_{\text{bat}}$ is the potential energy associated with the battery. The total potential energy for the system can be expressed in different forms depending the choice of state variable for the circuit, as in (19a) and (19b):

$$G[n, \Delta U] = F_e[n] + C[n] \left[ \frac{1}{2} (\Delta U)^2 - V \Delta U \right], \quad G[n, Q] = F_e[n] + \frac{1}{2} C[n]^{-1} Q^2 - VQ.$$  

In either case, equilibria are locally minimizing with respect to the pair $(n, \Delta U)$ or $(n, Q)$.

In order to transform $G$ into the form $F$ above, one must assume (1) either a static electric field or an electric field that adjusts instantaneously to any changes in $n$ (so that $\text{curl } E = 0$ and $E = -\nabla U$) and (2) either equilibrium conditions in the circuit (no current) or a circuit that adjusts instantaneously to any changes in the capacitance of the cell (so that $\Delta U = V$ and $Q = CV$ at all times). In §4.3 we have described how $G$ above can be transformed to $F$ if one makes these assumptions (and also employs the constitutive assumption $D = \epsilon(n) E$), the main points being that $E = -\nabla U$ and $\text{div } D = 0$ imply

$$Q \Delta U = \int_\Omega (D \cdot E) dV,$$

$\Delta U = V$ gives

$$E_{\text{cap}} + E_{\text{bat}} = \frac{1}{2} QV - QV = -\frac{1}{2} QV = -\frac{1}{2} \int_\Omega (D \cdot E) dV,$$

and $D = \epsilon(n) E$ and $E = -\nabla U$ give

$$-\frac{1}{2} \int_\Omega (D \cdot E) dV = -\frac{1}{2} \int_\Omega [\epsilon(n) \nabla U \cdot \nabla U] dV.$$  

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Thus $\mathcal{F}$ is not the appropriate free energy for modeling dynamics that include the coupled evolution of the electric field in the cell or the charge dynamics of the electric circuit. The potential energy $\mathcal{G}$, on the other hand, is valid in the absence of any of these equilibrium or instantaneous-adjustment assumptions.

The time scales for the various dynamic processes in our system vary widely and depend on details of any specific experiment being modeled. At one end of the spectrum is the switch-off time ($\tau_K$ in our notation, the slowest time scale, of the order of $10^{-2}$ s). At the other end is the time scale for the evolution of the electric field in the cell, $\tau_E$, governed by the time-dependent Maxwell equations, which is of the order of $10^{-13}$ s for the kinds of systems of interest to us. In between these extremes are the switch-on time, $\tau_V$, and the time scale for the dynamics of the electric circuit, $\tau_\sigma$. The switch-on time $\tau_V$ is proportional to $1/V^2$ (where $V$ is the applied voltage) and can vary from values comparable to $\tau_K$ to values of the order of $10^{-8}$ s. There is some overlap between values that $\tau_V$ can take and those that $\tau_\sigma$ can take, and our modeling has been concerned with such situations. The evolution of the electric field in the cell is several orders of magnitude faster than any of these, and its response has been treated as instantaneous, as is always assumed in modeling such systems.

For the example problem that we have analyzed in detail (a splay-Fréedericksz cell), the final form of the dynamical system (22) is quite clean, with everything given in simple explicit analytical expressions. This is, of course, a consequence of our modeling assumptions. The assumption that fields in the cell depend on only one space variable buys one a lot. It gives $D_z = \text{const}$ and $\sigma = \text{const}$ (in equilibrium) or $\sigma = \sigma(t)$ (in dynamics), and it enables us to write an explicit analytical expression for the capacitance of the cell, $C[n]$ in (14), and for the electric field in the cell, as in (5) and (8). If one abandons this assumption and allows fields in the cell to depend on more than one space variable, then all these consequences are lost. The assumption of fields depending on one space dimension is very common (and appropriate) in modeling thin-film liquid-crystal systems. The interplay between electric fields and liquid crystals has been of interest and importance ever since the discovery of the electro-optic effect in the 1970s—for an early review, see (10) and references therein. Bringing the electric circuit into the picture (as we have done here) has illuminated the role of the battery in producing the term $-\frac{1}{2}\epsilon(a)E \cdot n$ in the free energy (1), and it has highlighted what assumptions must be made to express the free energy in that form. If one merely wanted to obtain a coupled dynamical system such as (22), then one could have proceeded more directly, starting with appropriate equations for director dynamics and circuit dynamics

$$
\gamma \frac{\partial n}{\partial t} = \text{div} \left( \frac{\partial W_e}{\partial \nabla n} \right) - \frac{\partial W_v}{\partial n} + \lambda n + \epsilon_0 \sigma_a (E \cdot n) E, \quad R \frac{dQ}{dt} + \frac{1}{C} Q = V
$$

and coupling them via appropriate expressions for the electric field (which depends on $Q = \sigma A$, as in (5) and (8)) and the capacitance (which depends on $n$, as in (14)). Our more elaborated approach was motivated by a desire to see the “full picture” in terms of the potential energies, where they come from, and the assumptions needed for various simplifications and reductions.
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