

Critical point pairs for smectic-A* - smectic-C* phase transitions.

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Abstract

Liquid crystals is a class of materials possessing properties from both solids and fluids. Similar to solids the molecules arrange themselves in some sort of order. In the liquid crystal state there are multiple phases, smectic being one of them. In a smectic liquid crystal the molecules are arranged (along z) in layers. Of the smectic liquid crystals there exists different phases. In the smectic-A (Sm-A) phase the average tilt is 0 relative to z and in the Smectic-C (Sm-C) phase the average tilt is non-zero relative to z . Normally the liquid crystal will transition between the two phases by altering the temperature. In chiral smectics (i.e. Sm-A*, Sm-C*) it is possible to induce director tilting (i.e. the Sm-C* phase) from the Sm-A* phase via the application of an electric field. This is known as the bulk electroclinic effect (BECE). Also possible to have high-tilt - low-tilt Sm-C* transition, analogous to liquid-gas transition. Like liquid-gas transition, there is a critical point. We investigate possibility of high-tilt - low-tilt phase boundary with **two** critical points, one at each end of the boundary.

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1 Liquid Crystals: A brief overview

The phases of matter familiar to most people are gas, liquid, and solid. However, more than these three phases of matter exists. Liquid crystal are an intermediate phase present in certain material between the liquid and solid phase. To understand why liquid crystal is classified as a different phase we need to first look at the differences between liquids and solids. For a solid the position and orientation of the molecules are essentially fixed. In a liquid, the molecules are both free to move about and orient in any direction. A liquid crystal possess some properties of a solid while still remaining in a state very similar to that of a liquid. The molecules have a weak or no positional order and are free to move about like a liquid but they possess a preferred orientational direction. The preferred orientational direction in a liquid crystal is due to their elongated molecular structure. This structure causes the molecules to on average be oriented along their long axis in the same direction. This direction can be described using a unit vector called the director \hat{n} .

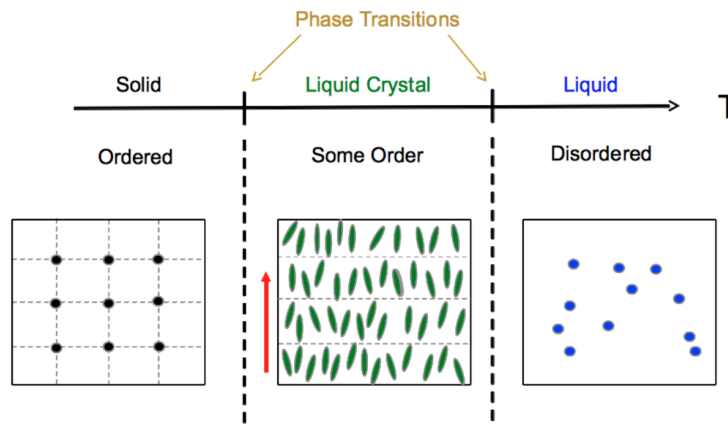


Figure 1: Liquid crystals are an intermediate phase of matter between a solid and liquid.

There are many different types of liquid crystals. The type we will analyze in this paper are thermotropic liquid crystals, which occur in specific temperature ranges. When the molecules display an orientational but no positional order the phase is called the nematic phase. This phase is usually found at high temperatures. As the temperature is decreased a positional order arises as seen in Fig 1. The molecules tend to be more likely to position themselves in different layers. This is the smectic class of phases and two of these smectic phases (Smectic-A and Smectic-C) will be studied in detail over the course of this paper.

2 Smectic-A to Smectic-C Transition

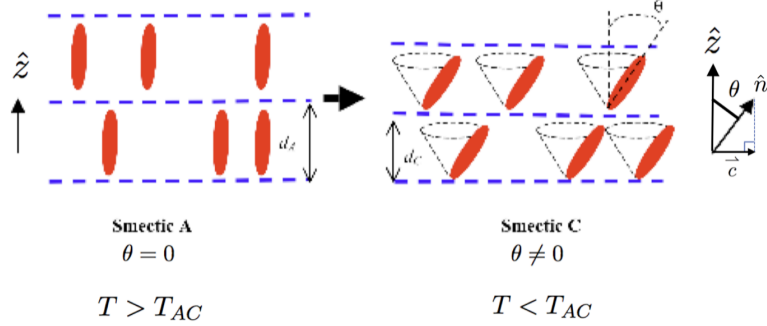


Figure 2: The differences between Sm-A phase and Sm-C phase are shown. On the far right, there is a geometrical interpretation of the order parameter vector c .

As seen in Fig. 2 the director \hat{n} of the liquid crystal in Smectic-A phase (Sm-A) is at a tilt of zero with respect to the smectic plane vector \hat{z} (i.e, $\theta = 0$) and the director of the Smectic-C (Sm-C) is at a tilt of non-zero with respect to \hat{z} ($\theta \neq 0$). This figure also demonstrate an orderparameter \vec{c} ($c = \sin(\theta)$) which is the projection of \hat{n} onto the layer. Where $c \neq 0$ or $\theta \neq 0$ characterizes the Sm-C transition. In this analysis only the magnitude of the vector is accounted for. Energetically, only the magnitude of the tilt matters and not the direction. This is why the free energy equation is in even powers of θ . We model the smectic liquid crystal system using the Landau Free Energy Equation:

$$F = \int dx dy dz [\frac{1}{2}r(T)\theta^2 + \frac{1}{4}u\theta^4 + \frac{1}{6}v\theta^6] = Vf(\theta) \quad (1)$$

where V is the volume of the system and $f(\theta)$ is used to model the free energy density of liquid crystal molecules in the absence of an electric field and is the following:

$$f(\theta) = \frac{1}{2}r(T)\theta^2 + \frac{1}{4}u\theta^4 + \frac{1}{6}v\theta^6 \quad (2)$$

- u is the quartic coefficient that will decide the nature of the transition between Sm-A and Sm-C phase that will occur. For $u < 0$ we will see the first order transition, for $u = 0$ the tricritical transition is exhibited and for $u > 0$ a continuous transition will occur.
- $r(T)$ is a function of temperature and will affect the positional order of the molecules in the liquid crystal. The function is of the form:

$$r(T) = \alpha(T - T_{AC}) \quad (3)$$

T_{AC} is the temperature where the transition between Sm-A and Sm-C occurs.

- $f(\theta) = \frac{1}{2}r(T)\theta^2 + \frac{1}{4}u\theta^4 + \frac{1}{6}v\theta^6$ is the free energy density of the system with $v \geq 0$, in order to maintain stability, i.e., to have a finite θ value.
- V is the volume of the system

2.1 Fixed points of the free energy function

The system will be the most stable in a low energy state. Therefore the preferred tilt of the molecules will be in local minimas of $f(\theta)$. To determine these stable points we will consider the following function:

$$\dot{\theta} = -\frac{df(\theta)}{d\theta} = -(r\theta \pm u\theta^3 + v\theta^5) \quad (4)$$

where the + corresponds to a value of $u > 0$ and the - corresponds to a value of $u < 0$.

2.1.1 Continuous transition: $u \geq 0$

For a continuous transition the θ^6 term is unnecessary for stabilization. so we will use $v = 0$ here to simplify the equation. By choosing $\dot{\theta} = 0$ we can solve for the stable points θ_* :

$$\begin{aligned} \dot{\theta} = 0 &= -\frac{df(\theta)}{d\theta} = -r\theta_* - u\theta_*^3 \\ \theta_* &= 0, \theta_* = \pm\sqrt{-\frac{r}{u}} \end{aligned} \quad (5)$$

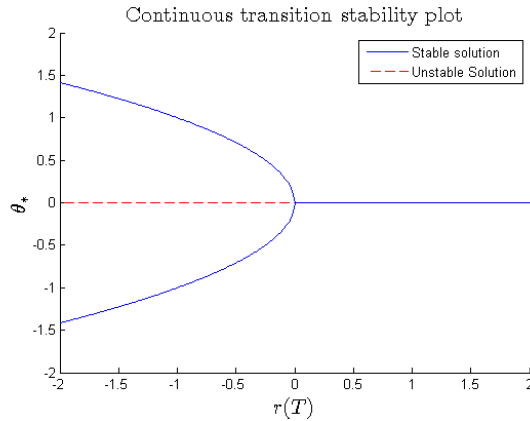


Figure 3: When T is reduced below T_{AC} ($r = 0$) the crystal continuously transitions into the Sm-C phase.

For any value of r a fixed point will exist on $\theta_* = 0$ but it is only stable for $r > 0$. The two points $\theta_* = \pm\sqrt{-\frac{r}{u}}$ are only real when $r < 0$ but they are always stable in that region. The progression of the stable points can be seen in Fig. 3. Whether or not a fixed point is stable depends on if the point is a local minima in the energy function. This can be determined by looking at the graphs in Fig. 4. This can be further seen in Fig. 5 where $\dot{\theta}$ is plotted against θ . For $r > 0$ the $\dot{\theta}$ -axis is only crossed once with a negative slope, meaning that the point is a stable fixed point. For $r < 0$ the $\dot{\theta}$ -axis is crossed three times, but here the origin is crossed with a positive slope so the point is unstable. The other two points are clearly stable as the slope is negative.

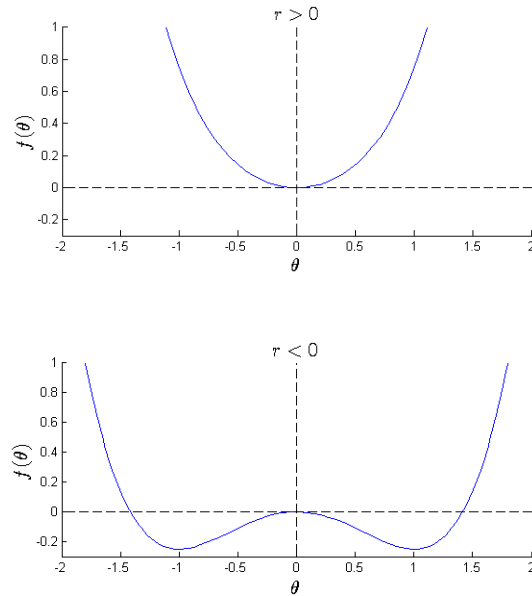


Figure 4: The free energy $f(\theta)$ plotted against θ for positive and negative r . The values: $u = 1$ and $r = \pm 1$ were used.

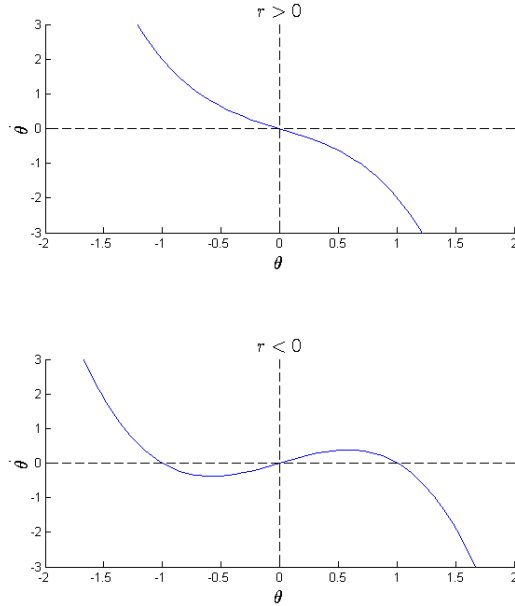


Figure 5: $\dot{\theta}$ plotted against θ for positive and negative r . The values: $u = 1$ and $r = \pm 1$ were used.

For $u > 0$ the phase transition is continuous. Recall that $r(T) = \alpha(T - T_{AC})$. From this it follows that $r > 0$ when the temperature T is: $T > T_{AC}$. The only stable value for $f(\theta)$ is when $\theta = 0$, the tilt is 0 and the liquid crystal is in the Sm-A phase. Now imagine we slowly reduce the temperature. At a certain point a tilt of the molecules will be energetically more favorable and a transition from Sm-A to Sm-C phase occurs. This threshold is exactly at: $r(T) = 0$, which is at the temperature: $T = T_{AC}$

2.1.2 First order transition $u < 0$

This case is more complicated than the previous one. A change in $r(t)$ will result in a much more dramatic effect on the tilt of the molecule. We can also no longer ignore the θ^6 term and we can't use $v = 0$, instead $v > 0$. $\dot{\theta}$ now becomes:

$$\dot{\theta} = -(r\theta - u\theta^3 + v\theta^5) \quad (6)$$

Solving for θ_* again yields us:

$$\theta_* = 0, \theta_* = \pm \sqrt{\frac{|u| \pm \sqrt{u^2 - 4rv}}{2v}} \quad (7)$$

This result shows us five possible fixed point values of θ_* . However, depending on the value of r certain points will appear and disappear in addition to changing their stability. A closer look of a few different values of r will give us

a better understanding on how the fixed points of the energy function changes depending on r . Each case is shown graphically in Fig. 6.

$r \leq 0$

In this range we have 3 solutions: $\theta_* = 0$, $\theta_* = \pm \sqrt{\frac{|u| + \sqrt{u^2 - 4rv}}{2v}}$.

The free energy plots (Fig. 6) reveals the stability for each fixed point in this case. The two non-zero points intercepts the θ -axis with a negative slope, which as stated before corresponds to a local minimum. Here the two minimas are identical, meaning the molecules are equally likely to tilt in either direction. Neither tilt is preferred. When $r = 0$ we get fixed points at: $\theta_* = 0$, $\theta_* = \pm \sqrt{\frac{u}{v}}$. Similar for when $r < 0$ the fixed point at the origin is unstable while the non zero points are stable. We can see that the maxima in the origin is starting to flatten out. We will see an additional two fixed points forming close to the origin as r increases.

$0 < r < \frac{3u^2}{16v}$

The fixed points are: $\theta_* = 0$, $\theta_* = \pm \sqrt{\frac{|u| \pm \sqrt{u^2 - 4rv}}{2v}}$ for a total of 5 fixed points.

By analyzing the free energy plots we notice that the line intercepts the θ -axis with a negative slope. The fixed point at the origin is stable. However, the two non-zero minimas are more favorable and the system is at the preferred Sm-C phase. We say preferred because the solution $\theta_* = 0$ is a stable solution. While the system is stable with no tilt, the system like any other will exhibit behavior that uses the least energy. Thus the non-zero solutions are preferred. If the system is found to have no tilt, that is its in the Sm-A phase the system is locally stable but more possible states exists. We call this kind of state a meta-stable state. The reason why the system is even able to be in Sm-A phase for this temperature range is because of the energy humps that exists between the zero and non-zero tilt states (this can be seen in Fig. 6). This hump acts like an energy barrier that needs to be surmounted in order for the transition to happen. This behavior is analogous to the super cooling of water. Super cooling is the process of cooling water below its freezing point without the liquid becoming a solid. The water is in a meta stable state. By adding a bit of energy to allow the water to overcome the energy barrier and the transition can happen. This can be done by tapping the container that holds the water or slightly stirring it. When the transition do happen it spreads out across the system so even if a small part of the crystal recieves the “energy boost” the transition is likely to spread across the entire system.

$r = r_T = \frac{3u^2}{16v}$ The solutions in this case are nearly identical to the previous case. What’s different here is that all three minimas are equally likely to occur. At exactly this temperature neither Sm-A or Sm-C are preferred. This value of r is the threshold where the preferred state of the system changes. This is an important threshold. We denote this specific value of r : r_T .

$$\frac{3u^2}{16v} < r < \frac{u^2}{4v}$$

The solutions in this case remains the same, but the behavior is similar to the $0 < r < r_T$ case. The system can be in a meta-stable. But at this range Sm-A is the more preferred state since the non-zero solutions now has a higher energy level compared to the Sm-A state. This is analogous to the super heating of water, very similar to the super cooling of water described earlier, but instead of cooling it below freezing, the water is now raised above its boiling temperature.

$$r \geq \frac{u^2}{4v} = r_u$$

At $r = \frac{u^2}{4v}$ we reach a second threshold. We have three fixed points at: $\theta_* = 0, \theta_* = \pm\sqrt{\frac{u}{2v}}$ instead of the five we had previously. The phase portrait tells us that the two non-zero solutions never intercepts the $\dot{\theta}$ -axis fully and are therefore only semi-stable fixed points with only the solution at the origin that is stable. This is an important threshold. We denote this specific value of r : r_u . For $r > r_u$ we only have one solution: $\theta_* = 0$. This is now the systems only fixed and stable point. This tells us that values of r in this range can't be in any other state than the Sm-A phase.

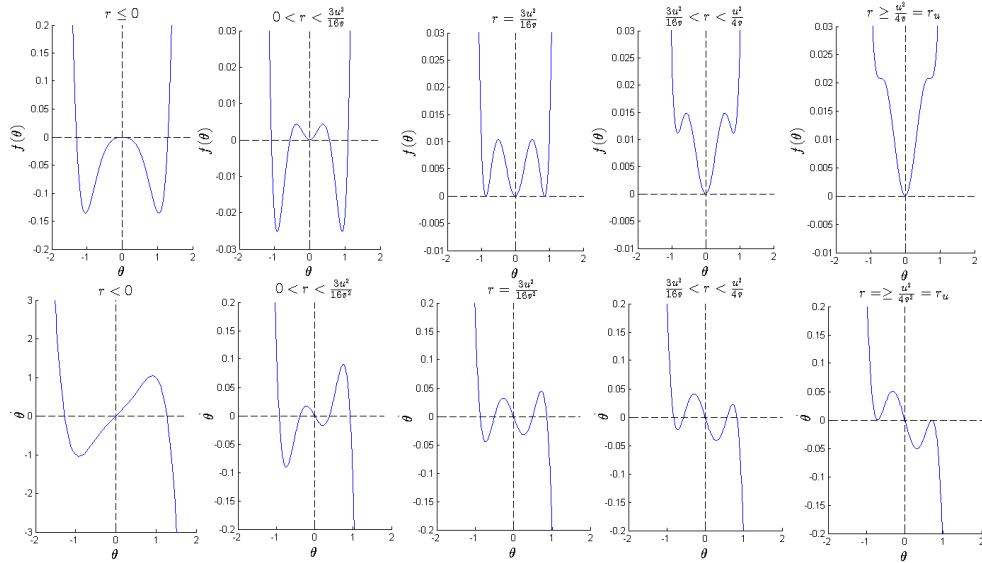


Figure 6: $f(\theta)$ plotted against θ for different values on r with it's corresponding stability plot under it. A negative slope when crossing the θ axis tells us that the specific fixed point is stable.

It is clear that the first order transition is more complicated than the continuous one. This is because the transition experiences a subcritical pitchform bifurcation. To get a better understanding of the transtion we can look at Fig. 7. implying that in regions where multiple stable solutions coexist, there is the

$r \leq 0$	3 possible fixed points. $\theta_* = \pm\sqrt{\frac{ u +\sqrt{u^2-4rv}}{2v}}$ and $\theta_* = 0$
$0 < r < \frac{u^2}{4v}$	5 possible fixed points. $\theta_* = \pm\sqrt{\frac{ u \pm\sqrt{u^2-4rv}}{2v}}$ and $\theta_* = 0$
$r = \frac{u^2}{4v}$	3 possible fixed points. $\theta_* = \pm\sqrt{\frac{ u }{2v}}$ and $\theta_* = 0$
$r > \frac{u^2}{4v}$	1 possible fixed point. $\theta_* = 0$

Table 1: Locations where the number of fixed points changes

possibility for hysteresis, or jumps, as the temperature parameter r is lowered. Consequently this means that the transition from Sm-A phase to Sm-C phase will be dramatic and not smooth like the continuous transition. There's a specific transition temperature, T_{AC} , where if $T > T_{AC}$ the system will always be in the Sm-A phase, but if $T < T_{AC}$ it can either be in the Sm-A phase or the Sm-C phase. The bifurcation diagram below demonstrates this.

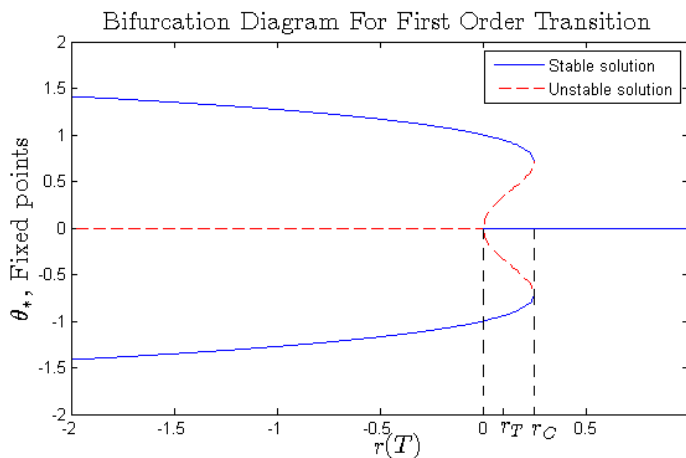


Figure 7: This diagram demonstrates how the number of solutions and their location changes depending on r . $u = -1$ and $v = 1$ were used here.

We can see in Fig. 7 that there's a transition temperature T_{AC} , where if $T > T_{AC}$ the system is in the Sm-A phase, but if $T < T_{AC}$ the system can be in either the Sm-A phase or the Sm-C phase. Another important thing to notice is that the critical temperature T_c ($r = 0$) lies below the transition temperature T_{AC} . This demonstrates that it is possible in a first order transition to be below the transition temperature but still exhibit the Sm-A phase.

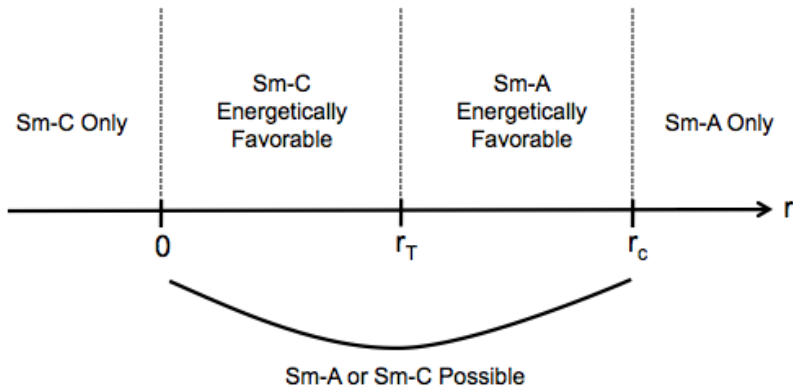


Figure 8: A 1-dimensional phase diagram of the transition.

The diagram above shows us a 1-dimensional phase diagram of the transition. It shows us that there's a region where both phases are possible with a threshold value $r_T = \frac{3|u|^2}{16v}$ where if $r > r_T$ Sm-A is more favorable and if $r < r_T$ Sm-C is more favorable.

Throughout the previous section, we have seen that smectic liquid crystals will undergo a phase transition from an average tilt of zero, to a nonzero tilt throughout. This happens by lowering the temperature of the system to some value of T_c . In a continuous phase transition, we see a supercritical pitchfork bifurcation at this critical point. The tilt of the molecules gradually increases as we lower temperature past this point. In a first order transition, we see the potential for hysteresis and a spontaneous jump in the tilting of the molecules near T_c , as is characteristic of a subcritical pitchfork bifurcation. In the next section, we will see how the application of an electric field can induce similar tilting behaviors in a liquid crystal cell while temperature is held constant. We will do this in a more quantitative way, whereas this section was meant to introduce the basic mathematical behavior of these phase transitions.

3 Induced tilt with an electric field

When an external electric field is applied to a chiral liquid crystal a tilt is induced. This is because chiral liquid crystals are ferroelectric. We denote the ferroelectric liquid crystals with a *, so ferroelectric Sm-A = Sm-A* and ferroelectric Sm-C = Sm-C*. This means that if we have a smectic liquid crystal in the Sm-A* phase we can use an electric field to induce a tilt and thus changing it's phase to Sm-C* without changing the temperature.

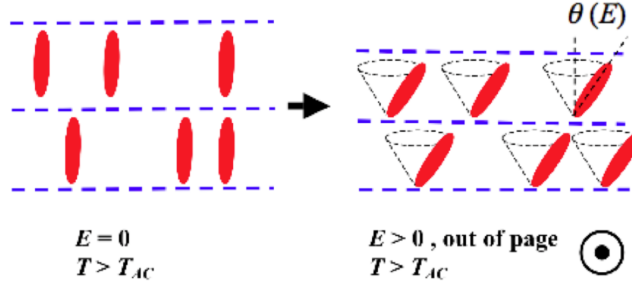


Figure 9: Applying an electric field E the liquid crystal transitions from Sm-A* to Sm-C* while the temperature remains above T_{AC} .

We expand the Landau Free Energy equation to include the external electric field, \vec{E} :

$$f(\theta) = \frac{1}{2}r(T)\theta^2 + \frac{1}{4}u\theta^4 + \frac{1}{6}v\theta^6 - E\theta \quad (8)$$

Through minimization of the energy equation with respect to θ we can solve for E and get:

$$E(\theta) = r(T)\theta + u\theta^3 + v\theta^5 \quad (9)$$

3.1 Continuous transition, $u > 0$

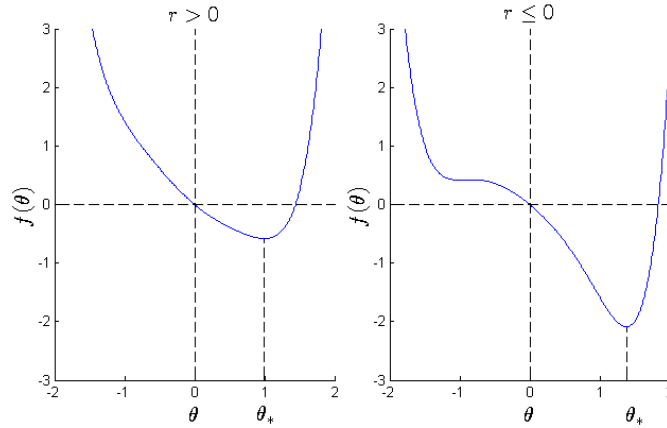


Figure 10: The free energy plot against θ with the an electric field applied to the crystal causing a tilt. $r \pm 1$, $u = 1$, $v = 1$ and $E = 1$

For the continuous transition we will only ever have one stable solution if an external electric field is applied. The continuous transition is therefore of little

interest to us for our analysis. A much more interesting development of the transition happens with $u < 0$.

3.2 First order transition, $u < 0$

Just like the previous section the first order transition is more interesting and complex than the continuous one. We begin with studying the θ vs $E(\theta)$ graph given by Eq. 9:

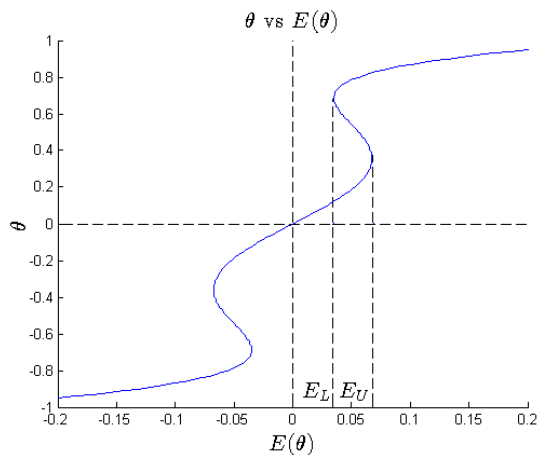


Figure 11: An 'S'-shape is clearly visible. $r = 0.3, u = -1, v = 1$. The value of r was chosen so it was within the multivalued region of Fig. 7.

In Fig. 11 we can see that for certain magnitudes of the electromagnetic field we have two possible solutions for θ . The 'S'-shape will only appear if $r(T)$ lies within the multivalued region seen in Fig. 7. This specific region is important to us because of the implications that comes with the 'S'-shape. It follows that there's at least two possible stable angles the molecules can be in and we will have a possible phase transition. In Fig. 12 I've plotted the free energy with an electric field of 0.05. I chose this value because it lies within the 'S'-shape of Fig. 11.

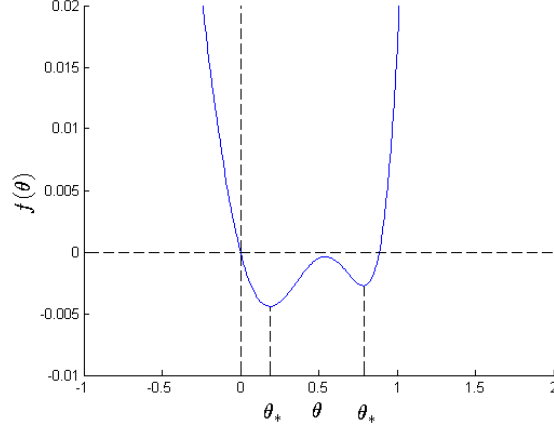


Figure 12: Because E lies within the ‘S’-region we have two stable solutions. $r(T) = 0.3, E = 0.05$.

$\theta(E)$ is only multivalued in a special region of r and E . To explore this we begin with minimizing $E(\theta)$ with respect to θ and looking at the numbers of solutions depending on r .

$$\frac{dE(\theta)}{d\theta} = r + 3u\theta^2 + 5v\theta^4 = 0 \quad (10)$$

$$\theta_* = \pm \frac{1}{10} \frac{\sqrt{10v(-3u \pm \sqrt{-20rv + 9u^2})}}{v} \quad (11)$$

It’s when we have 4 possible solutions for θ_* that we get the ‘S’-shape. This is only true when the following requirements are met:

- $u < 0$, first order transition is required.
- $r(T) < r_c = \frac{9u^2}{20v}$, second rootsign must remain real

With this we can find $E_{Upper}(\theta)$ and $E_{Lower}(\theta)$ by inserting the Eq. 11 into the $E(\theta)$, Eq. 9. This shows us the region of r where two stable solutions will be available. This is shown in fig. 13.

$$E_L(r) = \left(\sqrt{-\frac{3u}{10v} - \sqrt{\frac{9}{100}\left(\frac{u}{v}\right)^2 - \frac{r}{5v}}} \right) \left(-\frac{2}{5}u \sqrt{\frac{9}{100}\left(\frac{u}{v}\right)^2 - \frac{r}{5v}} + \frac{4}{5}r - \frac{3u^2}{25v} \right) \quad (12)$$

$$E_U(r) = \left(\sqrt{-\frac{3u}{10v} + \sqrt{\frac{9}{100}\left(\frac{u}{v}\right)^2 - \frac{r}{5v}}} \right) \left(+\frac{2}{5}u \sqrt{\frac{9}{100}\left(\frac{u}{v}\right)^2 - \frac{r}{5v}} + \frac{4}{5}r - \frac{3u^2}{25v} \right) \quad (13)$$

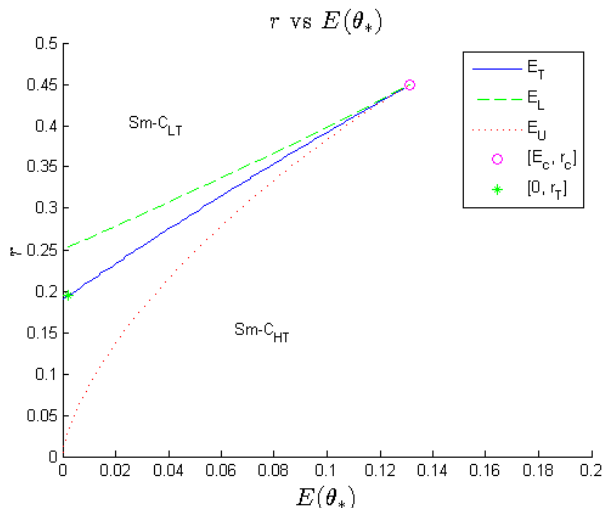


Figure 13: If $r(T)$ falls within the region between the red and blue line two stable solution will be available. r_T is the transition temperature for a system without an electric field and r_c is the critical point of the system. $u = -1, v = 1$.

For a system without an electric field we know that the transition is at $r = r_T = \frac{3u^2}{16v}$. But as soon as we apply an electric field the temperature for the transition changes. It is important for our analysis to know the required electric field for each value of $r(T)$ where the transition happen. An important note to make is that as soon as we add an electric field the system can never truly exist in the Sm-C* phase as a tilt will always be induced. Instead we will call it the low tilt Sm-C* phase (Sm-C*_{LT}) and the previous Sm-C* phase will be called high tilt Sm-C* phase (Sm-C*_{HT}). While we can't find this transition line analytically we can find it numerically using MATLAB. We do this by starting at $r(T) = r_T = \frac{3u^2}{16v}$ and slowly increase E until the two stable points are equally energetically favorable. For the starting case the electric field is as mentioned earlier 0. But as we increase $r(T)$ the required electric field also increases. If we look at at Fig. 12 we can see two stable points. But the first one is more energetically favorable than the second. However, if we increase the strenght of the electric field the second stable point will eventually become energetically favorable instead, this is when the transition occurs. We will keep repeating this process, slowly tracing out the transition line. Eventually $r(T)$ reaches a value above the blue line $r_u = \frac{u^2}{4v}$ if $E = 0$. At this location the second stable point cease to exist and only the low tilt Sm-C* phase is available. But if we increase the electric field it will reappear once we cross the blue line. When we finally reach $r(T) = r_c = \frac{9u^2}{20}$ we have reached the critical point of the system and we can't continue further since there's no longer a clear transition happening. The zero-field Sm-A* - Sm-C* phase transition corresponds to moving up/down on the vertical (i.e., r) axis. The 1st order transition occurs at $r = \frac{3u^2}{16v}$ m i.e., where

the transition line intersects the vertical axis. Moving around the critical point is analogous to moving around the liquid-gas critical point. There won't be a clear transition between the Sm-C_{LT}^* phase and Sm-C_{HT}^* phase just as there's no clear difference between the liquid and the gas as they are both fluids and symmetrically similar. We call the traced out line E_T and it can be seen in Fig. 14.

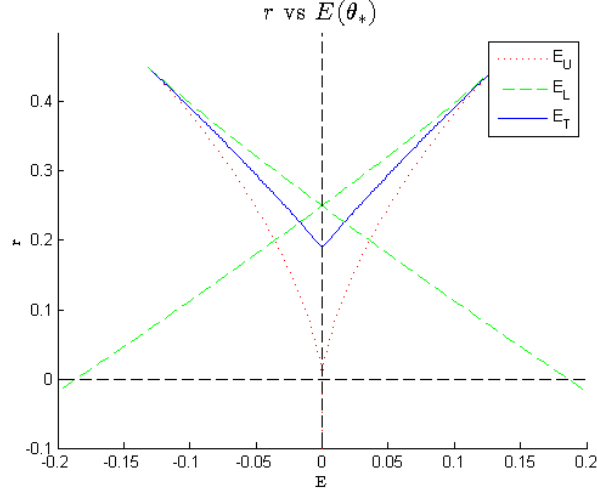


Figure 14: Choosing a location inside E_U and E_L is analogous to the 'S'-region seen in Fig. 11. $u = -1, v = 1$.

Fig. 14 is from a MATLAB program included in the appendix. It will allow you to explore interactively by choosing a value of E and $r(T)$ by clicking the graph which the program then uses to plot the energy density function. Playing around with it will help you understand how the stable points changes depending on whether we are outside or inside the red and blue line. It also shows how the negative electric field affects the system by crossing over to the positive side.

4 Including the effects of polarization

So far we have used a very simplified model. A more complete model of the energy density function contains a polarization variable ' p '.

$$f(\theta, p) = \frac{1}{2}r_\theta\theta^2 + \frac{1}{4}u_\theta\theta^4 + \frac{1}{6}v_\theta\theta^6 + \frac{1}{2}r_p p^2 + \frac{1}{4}u_p p^4 + \frac{1}{6}v_p p^6 - Ep - ep^2\theta^2 - \gamma\theta p \quad (14)$$

Our initial goal here is to transform the function to something similar to what we've been working with in the previous sections. To do this we will minimize the function by differentiating with respect to θ and then setting it equal to 0. This allows us to solve for p_{min} in terms of θ .

$$\frac{df(\theta, p_{min})}{d\theta} = r_\theta \theta + u_\theta \theta^3 + v_\theta \theta^5 - 2ep_{min}^2 \theta - \gamma p_{min} = 0 \quad (15)$$

$$p_{min} = \frac{-\gamma + \sqrt{8e\theta^6 v_\theta + 8e\theta^4 u_\theta + 8e\theta^2 r_\theta + \gamma^2}}{4e\theta} \quad (16)$$

Our next step is to solve for the electric field E . We can do this by differentiating the energy density with respect to p and then minimizing it.

$$\frac{df(\theta, p)}{dp} = r_p p + u_p p^3 + v_p p^5 - E - 2ep\theta^2 - \gamma\theta = 0 \quad (17)$$

$$E = r_p p + u_p p^3 + v_p p^5 - 2ep\theta^2 - \gamma\theta = 0 \quad (18)$$

Inserting p_{min} (Eq. 14) into Eq. 16 followed by expanding it with respect to θ to the fifth power we get the following expression:

$$\begin{aligned} E = & \left(\frac{r_p r_\theta - \gamma^2}{\gamma} \right) \theta + \\ & \left(\frac{u_p r_\theta^3 + r_p u_\theta \gamma^2 - 2er_\theta \gamma^2 - 2r_p e r_\theta^2 - 2er_\theta \gamma^2}{\gamma^3} \right) \theta^3 + \\ & \left(\frac{v_p r_\theta^5 - 2eu_\theta \gamma^4 + 4e^2 r_\theta^2 \gamma^2 + 3u_p r_\theta^2 u_\theta \gamma^2 - 6u_p r_\theta^4 e + r_p v_\theta \gamma^4 - 4r_p e r_\theta u_\theta \gamma^2 + 8r_p e^2 r_\theta^3}{\gamma^5} \right) \theta^5 + \\ & O(\theta^7) \end{aligned} \quad (19)$$

The last step to make it similar to Eq. 9 is to replace the parameters before each θ with new parameters, ' a, b, c '.

$$E(a, b, c) = a\theta + b\theta^3 + c\theta^5 \quad (20)$$

With a, b, c defined as:

$$\begin{aligned} a &= \frac{r_p r_\theta - \gamma^2}{\gamma} \\ b &= \frac{u_p r_\theta^3 + r_p u_\theta \gamma^2 - 2er_\theta \gamma^2 - 2r_p e r_\theta^2 - 2er_\theta \gamma^2}{\gamma^3} \\ c &= \frac{v_p r_\theta^5 - 2eu_\theta \gamma^4 + 4e^2 r_\theta^2 \gamma^2 + 3u_p r_\theta^2 u_\theta \gamma^2 - 6u_p r_\theta^4 e + r_p v_\theta \gamma^4 - 4r_p e r_\theta u_\theta \gamma^2 + 8r_p e^2 r_\theta^3}{\gamma^5} \end{aligned} \quad (21)$$

Our energy function now has the exact same form as the previous more simpler model. But unlike the previous one all three parameters depend on the temperataure coefficient r_θ . This proves to be very important as it may mean the θ vs E can start with no 'S'-shape, that is no possible coexistence and

no $\text{Sm-C}_{LT}^*-\text{Sm-C}_{HT}^*$ transition as E is varied. But as the temperature lowers an ‘S’-shape might appear which means the crystal is in it’s Sm-C_{HT}^* phase (the ‘S’-shape can be seen in Fig. 11). Followed by the crystal reverting back to it’s Sm-A^* shape and the ‘S’-shape vanishing. A behaviour that would be impossible with our previous more simpler model which can be seen in Fig. 13. Fig. 15 below is what this new model’s a vs $E(\theta_*)$ graph could look like which is analogous to what’s seen in Fig. 13. Note that the transition line no longer intersects the vertical axis. This means that the zero-field transition would be continuous.

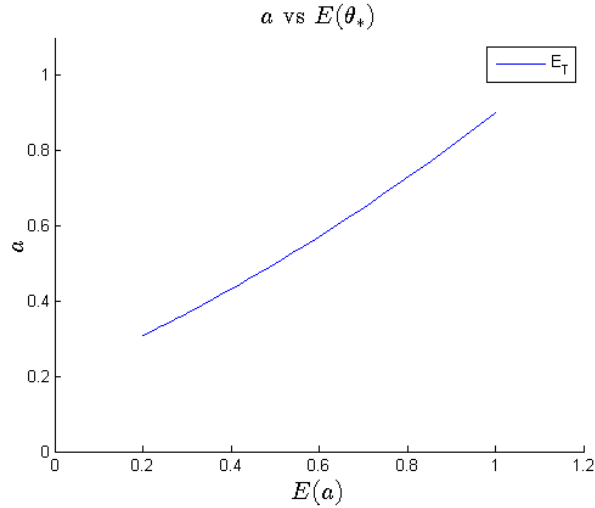


Figure 15: Mockup of how we imagine the E_T line to look like with polarization added to our model.

What is different here compared to what we found with our previous model is two critical points instead of one. This is a consequence of adding polarization to the model. Our next and final step in our analysis is to find a numerical value of the parameters to prove that this phenomenon is possible.

5 Sm-A^* to Sm-C^* transition.

By expressing r_θ in terms of a we can effectively eliminate r_θ from our expressions. We now have a as the temperature coefficient which will change the current state of the crystal similar to how we varied $r(T)$ earlier.

$$r_\theta = \frac{\gamma(\gamma + a)}{r_p} \quad (22)$$

By inserting this in to b and c we get the following two expressions:

$$\begin{aligned}
B(a) &= b_0 + b_1 a + b_2 a^2 + b_3 a^3 \\
C(a) &= c_0 + c_1 a + c_2 a^2 + c_3 a^3 + c_4 a^4 + c_5 a^5
\end{aligned} \tag{23}$$

With the coefficients in front of the powers of a being:

$$\begin{aligned}
b_0 &= \frac{\gamma^2 r_p^4 u_\theta + \gamma^6 u_p - 4e\gamma^4 r_p^2}{\gamma^3 r_p^3} \\
b_1 &= \frac{3\gamma^5 u_p - 6e\gamma^3 r_p^2}{\gamma^3 r_p^3} \\
b_2 &= \frac{3\gamma^4 u_p - 2e\gamma^2 r_p^2}{\gamma^3 r_p^3} \\
b_3 &= \frac{u_p}{r_p^3} \\
c_0 &= \frac{6e\gamma^4 u_\theta r_p^5 - 12e^2 \gamma^6 r_p^3 + 6e\gamma^8 u_p r_p - \gamma^4 r_p^6 v_\theta - 3\gamma^6 u_\theta u_p r_p^3 - \gamma^{10} v_p}{\gamma^5 r_p^5} \\
c_1 &= \frac{e\gamma^3 u_\theta r_p^5 - 32e^2 \gamma^5 r_p^3 + 24e\gamma^7 u_p r_p - 6\gamma^5 u_\theta u_p r_p^3 - 5\gamma^9 v_p}{\gamma^5 r_p^5} \\
c_2 &= \frac{36e\gamma^6 u_p r_p - 28e^2 \gamma^4 r_p^3 - 3\gamma^4 u_\theta u_p r_p^3 - 10\gamma^8 v_p}{\gamma^5 r_p^5} \\
c_3 &= \frac{24e\gamma^5 u_p r_p - 8e^2 \gamma^3 r_p^3 - 10\gamma^7 v_p}{\gamma^5 r_p^5} \\
c_4 &= \frac{6e\gamma^4 u_p r_p - 5\gamma^6 v_p}{\gamma^5 r_p^5} \\
c_5 &= \frac{v_p}{r_p^5}
\end{aligned} \tag{24}$$

5.1 Requirements

We now have everything we need for our analysis. For the transition to be possible we need to fulfil a set of requirements. All the requirements has already been mentioned in section 2 and 3 but we will go through them again with our new updated model.

In order for the crystal to experience a first order transition we showed that u must be less than 0. Translating this to our current model we get the following requirement:

$$B(a) < 0 \tag{25}$$

In addition to this, we want it to be at a positive value at $a = 0$ this is because we need the crystal to experience a continuous transition at $E = 0$ which can

only happen if $B(0) > 0$ (analogous to $u > 0$). But with our current model it is possible for $B(a)$ to vary between a positive and negative value. What we are looking for is a region where $B(a)$ is less than zero.

In order for our energy function to be stable $C(a)$ must be positive. This is because for high θ s the $\frac{1}{6}C(a)\theta^6$ term will dominate. If $C(a)$ is negative at any point the potential will approach negative infinity which we must avoid. Therefore we obtain our second requirement:

$$C(a) > 0 \quad (26)$$

Our fourth and final requirement are obtained from Eq. 11, the fixed points for θ . Which in our current model looks like:

$$\theta_* = \pm \frac{1}{10} \frac{\sqrt{10C(a)(-3B(a) \pm \sqrt{-20aC(a) + 9B(a)^2})}}{v} \quad (27)$$

In order for a second stable point to exist it is crucial that all five fixed points are real. We are therefore met with the following requirement:

$$R(a) = B(a)^2 - \frac{20}{9}aC(a) > 0 \quad (28)$$

Defining the restricted function as $R(a)$.

In order for the ‘S’-shape to appear in the E vs θ graph the following requirements must be met:

1. $B(0) > 0$ To get a continuous transtion at $E = 0$.
2. $B(a) < 0$ This allows the crystal to experience a first order transition.
3. $C(a) > 0$ Necessary for the system to be stable.
4. $R(a) > 0$ Necessary for the 2-phase coexistence and possibility of Sm- C_{LT}^* - Sm- C_{HT}^* transition. Must be true in a common region with the second requirement.

5.2 Finding a numerical solution

Ideally we would try to find an analytical solution to our problem. But it’s not possible for this case. However, we can find a numerical solution thus proving it is possible. We do this by first simplifying the function using already known restriction. These restriction are directly derived from our requirements explained above.

- $B(0) = b_0 > 0$

- $c_0 > 0$
- $c_5 > 0$ This and the previous restriction is true because of the third requirement.

We can take advantage of this by expressing the other coefficients in terms of b_0, c_0 and c_5 . As it turns out solving for b_3 and expressing the other coefficients in terms of it will make it easier to work with, even if we have no actual restriction on b_3 . I chose to replace u_θ with b_0 , u_p with b_3 , v_θ with c_0 and v_p with c_5 After inserting everything into Eq. 22. we get:

$$\begin{aligned}
b_0 &= b_0 \\
b_1 &= 3\gamma^2 b_3 - \frac{6e}{r_p} \\
b_2 &= 3\gamma b_3 - \frac{2e}{r_p \gamma} \\
b_3 &= b_3 \\
c_0 &= c_0 \\
c_1 &= \frac{4eb_0 3r_p^3 - 16e^2 r_p^2 - 4\gamma^2 e u_p - 6\gamma b_3 b_0 r_p^4 + 6\gamma^4 b_3 u_p r_p + 5\gamma^4 c_5 r_p^4}{r_p^4} \\
c_2 &= \frac{24\gamma^2 e b_3 r_p^2 - 28e^2 r_p - 3b_3 b_0 r_p^3 \gamma + 3\gamma^4 b_3 u_p + 10\gamma^4 c_5}{\gamma r_p^3} \\
c_3 &= \frac{24e b_3 r_p \gamma^2 - 8e^2 + 10\gamma^4 r_p^2 c_5}{\gamma^2 r_p^2} \\
c_4 &= \frac{6e b_3 + 5\gamma^2 c_5 r_p}{\gamma r_p} \\
c_5 &= c_5
\end{aligned} \tag{29}$$

We now have everything we need to come up with a possible numerical solution to our problem. We begin with listing the three restrictions we have:

- $b_0 > 0$ because of requirement 1.
- $c_0 > 0$ because of requirement 3.
- $c_5 > 0$ because of requirement 3.

There are multiple ways to do this. I choose to use MATLAB to bruteforce a solution since doing it analytically would be very difficult. This turns out to be a sufficient method and multiple solutions were found. The MATLAB program I used it included in the appendix. The way I set it up is simple. I choose a

value for b_0, b_3, c_0 and c_5 that was within their restrictions. I choose:

$$\begin{aligned} b_0 &= 1 \\ b_3 &= 0.3 \\ c_0 &= 1 \\ c_5 &= 1 \end{aligned} \tag{30}$$

This was mostly done arbitrarily. (The slightly lower b_3 results in more solutions). You could optimize the other coefficients and yield more solutions, but I deemed it unnecessary for this analysis. What's left is to find a numeric value for e, r_p and γ . This was done by continuously cycle each parameter from -1 to 1 in steps of 0.1 . During each cycle the program checks if there's a region where all requirements are met. Fig. 15 below is one example of a solution it found.

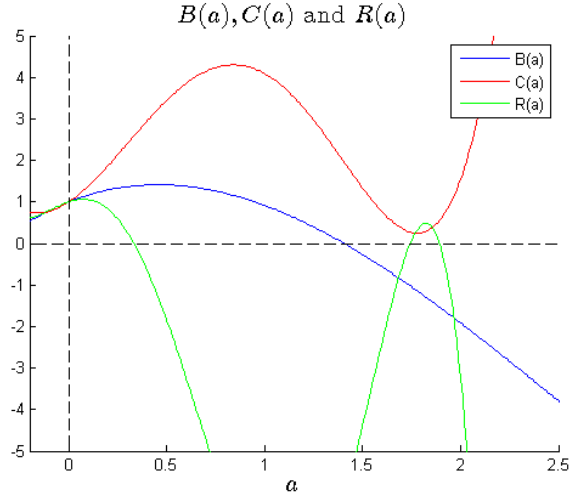


Figure 16: The region we are looking for is where $B(a)$ is negative and $R(a)$ is positive. Which we see a small region of here. $C(a)$ must also remain positive for $a > 0$.

The parameter values found displayed in Fig. 16 is:

$$\begin{aligned} e &= -0.30 \\ \gamma &= -0.30 \\ r_p &= 1.00 \\ u_p &= 0.30 \\ u_\theta &= -0.41 \\ v_\theta &= 0.97 \\ v_p &= -1.00 \end{aligned} \tag{31}$$

We can now show the phase transition going from $\text{Sm-}C_{LT}^*$ to $\text{Sm-}C_{HT}^*$ and back to $\text{Sm-}C_{LT}^*$ again as a gets lower.

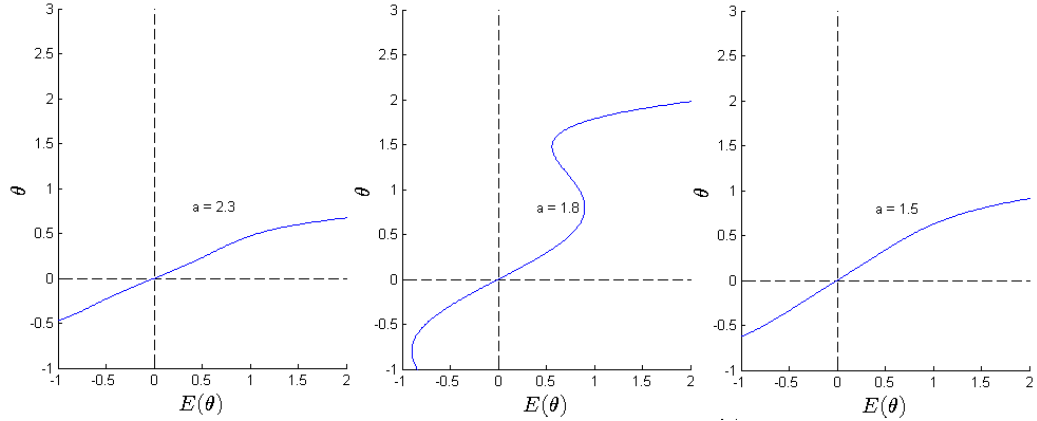


Figure 17: The generated θ vs $E(\theta)$ graph from Fig. 15. If we start with an a above the desired region no S-shape appears. But as a lowers the S appears and then disappears as we move outside the region again.

We now have everything we need to make the actual plot instead of the mockup in Fig. 15. We do this by looking at the energy density which now can be reduced to the following form:

$$f(\theta) = \frac{1}{2}a\theta^2 + \frac{1}{4}B(a)\theta^4 + \frac{1}{6}C(a)\theta^6 - E\theta \quad (32)$$

Using MATLAB we will now search for E_T by altering a and E respectively and looking for the transition. Just as we did previously with r and E . Fig. 18 below shows us our result.

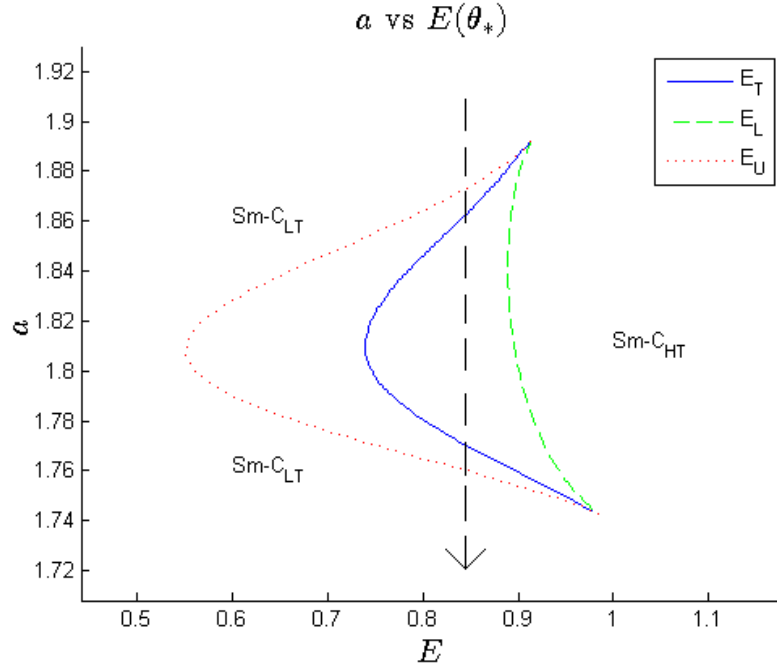


Figure 18: Instead of the nearly straight line we expected we got a ‘C’-shape. But we did find two critical points as expected.

While we expected a straighter line this doesn’t disagree with what we expected to find, two critical points. In the appendix the MATLAB program is included that was used to create Fig. 18. It also includes an interactive part similar to the program used to create Fig. 14. What we have found in our analysis proves the possibility of smectic liquid crystals having two critical points instead of one as previously believed. But the ‘C’-shape allows for reentrance. Consider a fixed E (i.e. moving along a vertical locus as seen in Fig. 18.) Move from high T (i.e. large a) to small T (i.e. small a). The liquid crystal experiences several transitions, $\text{Sm-C}_{LT}^* - \text{Sm-C}_{HT}^* - \text{Sm-C}_{LT}^*$. i.e., Sm-C_{LT}^* phase is reentered.

5.3 Future research

This analysis is not yet fully complete. There are many areas where this model can be developed. Example of such areas are the energy density function. We choose our model because of it’s simplicity which was suited for our analysis. Adding θp^3 and $\theta^3 p$ coupling terms would make the model more complete. Other possibilities include looking closer to the result seen in Fig. 18. The shape will change depending on the values of the parameters we use and it could be necessary to analyze its behaviour.

6 Appendix

```

%r_vs_E.m
%Ted Cassirer

%Run this program and wait a few seconds.
%When the graph pops up you can click in the graph and it will plot the
%free energy with the r and E you clicked on in the graph.
%To stop the program, just press a key on your keyboard while mousing over
%the graph. Might have to press twice

%The parameter values chosen here are v = 1 and u = -1
%Changing them might make the program to not work as some things here are
%explicitly coded for these values (Like starting point for finding
%the roots)

clf
clc
clear all
u = -1;
v = 1;

r_c = 9*u^2/(20*v);
r_u = u^2/(4*v);
r_lst = 3*u^2/(16*v);

E = @(r, c) (r*c + u*c.^3 + v*c.^5);
E_c = 1*(-3*u/(10*v))^0.5*(6/25*u^2/v);

a = @(r)(9/100*(u/v)^2-r/(5*v)).^0.5;

%E Lower
E_L = @(r)((-3*u/(10*v)-a(r)).^0.5*(-2/5*a(r).*u+4*r/5-3/25*u^2/v));

%E Upper
E_u = @(r)((-3*u/(10*v)+a(r)).^0.5*(2/5*a(r).*u+4*r/5-3/25*u^2/v));

f = @(r, c, E_m) (1/2*r.*c.^2 + 1/4*u*c.^4 + 1/6*v*c.^6 - E_m*c);
df = @(r, c, E_m) (r*c + u*c.^3 + v*c.^5 - E_m);

r_T = [];
E_T = [];
N = 100; %Step-count
rr = r_lst; %Value of r where it starts the search for r_T
for Ev = linspace(0, E_c, N)

    for rv = linspace(rr, r_c, N)

        if E_u(rv) < Ev && Ev < E_L(rv)
            c1 = fzero(@(c)df(rv, c, Ev), 0); %The minima in the middle c~0
            c2 = fzero(@(c)df(rv, c, Ev), 1); %The minima to the right c~1

            f1 = f(rv, c1, Ev);
            f2 = f(rv, c2, Ev);

```

```

    %r moves up. When the second minima is above the first we have
    %r_T. %Can make it more accurate but since this is just
    %graphics it wont make a difference really
    if f1 <= f2
        r_T = [r_T rv];
        E_T = [E_T Ev];
        rr = rv;
        break
    end
end
end
end

%The interactive part
figure(1);
r_vec = linspace(-0.2, 9/20, 100);
clf
hold on
plot(E_u(r_vec), r_vec, 'r:')
plot(E_L(r_vec), r_vec, 'g--')
plot(E_T, r_T)
plot(-1*E_L(r_vec), r_vec, 'g--')

plot(-1*E_u(r_vec), r_vec, 'r:')

plot(-E_T, r_T)
clc
plot([-1.5 1.5], [0 0], '--k')
plot([0 0], [-1 1], '--k')
legend('E_U', 'E_L', 'E_T')
title('$r$ vs $E(\theta)$', 'Interpreter', 'LaTeX', 'fontsize', 16)
xlabel('$E(\theta)$', 'Interpreter', 'LaTeX', 'fontsize', 16)
ylabel('$r$', 'Interpreter', 'LaTeX', 'fontsize', 16)
%Axis for the first plot. Change these values if you want to zoom in
axis([-0.2 0.2 -0.1 0.5])
xlabel('E')
ylabel('r')
while true

    figure(1);
    [x y] = ginput(1);
    figure(2);
    clf
    hold on

    %Finds the local minimas. It's sloppy, but it works well enough.
    c1 = fzero(@(c)df(y, c, x), -1);
    c2 = fzero(@(c)df(y, c, x), 1);
    c3 = fzero(@(c)df(y, c, x), 0);

    f1 = f(y, c1, x);
    f2 = f(y, c2, x);

```

```
f3 = f(y, c3, x);

plot(c1, f1, '*g')
plot(c2, f2, 'or')
plot(c3, f3, 'xm')

plot([-1.5 1.5], [0 0], '--k')
plot([0 0], [-1 1], '--k')
fplot(@(c) f(y, c, x), [-1.5 1.5 min([f1 f2 f3])-0.01 0.1])

xlabel('c')
ylabel('f')
if waitforbuttonpress
    break
end
end
```

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%This program searches for possible solutions described in section 5.2 When you start the program a window will quickly pop up showing you a possible solution and the program pauses. The corresponding parameter values will be displayed in the command window and saved to the array 'values'. If you want a different solution you can press any key to unpause the program and the program will start searching again for another solution and stopping again as soon as it find another solution.

```
f1 = figure(1);
```

```
%Defined parameters
```

```
b__0 = 1;
```

```
b3 = 0.3;
```

```
c0 = 1;
```

```
c5 = 1;
```

```
%Changes the range 'a' is changed between to look if the current cycle is a solution.
```

```
av = 0:0.1:4;
```

```
%e, gamma and r__p cycles between -1 and 1 to find possible solutions
```

```
for e = -1:0.1:1
```

```
    for gamma = -1:0.1:1
```

```
        for r__p = -1:0.1:1
```

```
            %Eq. 29
```

```
            b1 = -6*e/r__p+3*gamma^2*b3;
```

```
            b2 = -2*e/(gamma*r__p)+3*gamma*b3;
```

```
            c1 = -16*e^2/r__p^2-4*gamma^2*e*b3/r__p+4*e*b__0/ ...  
                (gamma*r__p)+6*gamma^4*b3^2-6*gamma*b3*b__0+5*gamma^4*c5;
```

```
            c2 = -28*e^2/(gamma*r__p^2)+24*gamma*e*b3/r__p+3*gamma^3* ...  
                b3^2-3*b3*b__0+10*gamma^3*c5;
```

```
            c3 = -8*e^2/(gamma^2*r__p^2)+24*e*b3/r__p+10*gamma^2*c5;
```

```
            c4 = 6*e*b3/(gamma*r__p)+5*gamma*c5;
```

```
            B = @(a) b__0 + b1*a + b2*a.^2 + b3*a.^3;
```

```
            C = @(a) c0 + c1*a + c2*a.^2 + c3*a.^3 + c4*a.^4 + c5*a.^5;
```

```
            R = @(a) B(a).^2-(20/9).*a.*C(a);
```

```
            a1 = 0:0.01:20;
```

```
%Checks if C(a) is positive for a>0 and if B(a) is negative at any point.
```

```
if C(a1)>0 & min(B(a1))< 0
```

```
    for a = av
```

```
        %Looks for a region where all requirements are met.
```

```
        if B(a) < 0 && R(a) > 0
```

```
            %A solution has been found is now plotted.
```

```
            clf
```

```
            hold on
```

```
            v = -2:0.01:8;
```

```
            plot(v,B(v))
```

```
            plot(v,C(v),'r')
```

```
            plot(v,R(v),'g')
```

```

plot([-10 10],[0 0],'--k')
plot([0 0],[-100 100],'--k')

xlabel('$a$', 'Interpreter', 'LaTeX', 'fontsize', 16)
legend('B(a)', 'C(a)', 'R(a)')
title('$B(a), C(a)$ and $R(a)$', 'Interpreter', ...
      'LaTeX', 'fontsize', 16)
axis([-0.2 4 -5 5])
drawnow

%All the parameter values are assigned to the
%solution that was found
['e r__theta r__p gamma u__p u__theta v__theta v__p']
values = num2cell([e, gamma*(gamma+a)/r__p , ...
  r__p, gamma, b3*r__p^3, -gamma*(b3*gamma^3 ...
  *r__p-b__0*r__p-4*e*gamma)/r__p^2, ...
  gamma*(3*b3^2*gamma^5*r__p^5+c5*gamma^5* ...
  r__p^5-3*b__0*b3*gamma^2*r__p^5-12*b3*e* ...
  gamma^3*r__p^4+6*b__0*e*r__p^4-c0*r__p^5+ ...
  12*e^2*gamma*r__p^3)/r__p^6, -c5*r__p^5])

[e, r__theta, r__p, gamma, u__p, u__theta, ...
  v__theta, v__p] = values{:};
pause

end
end
end
end
end
end
end
end

```

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```

%a_vs_E.m
%Ted Cassirer

%This program allows you to interactively experiment with Fig. 18 in the
%paper.
%Two window will pop up after a few seconds when you run this. In the first
%window you can click and the energy density will be plotted in window two
%with the choosen a and E value. When you are finished click in the command
%window and hold 'ctrl+C' or MATLAB might crash.

clear
clc
clf
%These are the values of the parameters found earlier. Also the same used
%in the paper
values = num2cell([ -0.3000    -0.4500    1.0000    -0.3000    ...
                   0.3000    -0.4104    0.9712    -1.0000]);

[e, r_theta, r_p, gamma, u_p, u_theta, v_theta, v_p] = values{:};

b__0 = -((4*e*gamma^4)/(r_p)-gamma^2*r_p*u_theta-(gamma^6*u_p)/ ...
         (r_p^3))/(gamma^3);
b__1 = -((6*e*gamma^3)/(r_p)-(3*gamma^5*u_p)/(r_p^3))/(gamma^3);
b__2 = -((2*e*gamma^2)/(r_p)-(3*gamma^4*u_p)/(r_p^3))/(gamma^3);
b__3 = (u_p)/(r_p^3);
c__0 = (-12*e^2*gamma^6/r_p^2+6*e*gamma^4*u_theta+6*e*gamma^8*u_p/ ...
        r_p^4-gamma^4*r_p*v_theta-3*gamma^6*u_theta*u_p/r_p^2- ...
        gamma^10*v_p/r_p^5)/gamma^5;
c__1 = (-32*e^2*gamma^5)/(r_p^2)+4*e*gamma^3*u_theta+(24*e*gamma^7* ...
        u_p)/(r_p^4)-(6*gamma^5*u_theta*u_p)/(r_p^2)-(5*gamma^9*v_p) ...
        /(r_p^5))/(gamma^5);
c__2 = (-28*e^2*gamma^4)/(r_p^2)+(36*e*gamma^6*u_p)/(r_p^4)-(3* ...
        gamma^4*u_theta*u_p)/(r_p^2)-(10*gamma^8*v_p)/(r_p^5))/(gamma^5);
c__3 = (-8*e^2*gamma^3)/(r_p^2)+(24*e*gamma^5*u_p)/(r_p^4)-(10* ...
        gamma^7*v_p)/(r_p^5))/(gamma^5);
c__4 = ((6*e*gamma^4*u_p)/(r_p^4)-(5*gamma^6*v_p)/(r_p^5))/(gamma^5);
c__5 = -(v_p)/(r_p^5);
B = @(a) b__0 + b__1*a + b__2*a.^2 + b__3*a.^3;
C = @(a) c__0 + c__1*a + c__2*a.^2 + c__3*a.^3 + c__4*a.^4 + c__5*a.^5;

f = @(theta, a, E) (1/2)*a.*theta.^2+(1/4)*B(a).*theta.^4+(1/6)*C(a).* ...
    theta.^6-E.*theta;

E__L = @(a) sqrt(-3*B(a)./(10*C(a))-sqrt((9/100)*(B(a)./C(a)).^2-a./ ...
    (5*C(a)))).*(-(2/5).*B(a).*sqrt((9/100).*(B(a)./C(a)).^2-a./ ...
    (5*C(a)))+(4/5)*a-(3/25)*B(a).^2./C(a));
E__U = @(a) sqrt(-3*B(a)./(10*C(a))+sqrt((9/100)*(B(a)./C(a)).^2-a./ ...
    (5*C(a)))).*((2/5).*B(a).*sqrt((9/100).*(B(a)./C(a)).^2-a./ ...
    (5*C(a)))+(4/5)*a-(3/25)*B(a).^2./C(a));

tv = -5:0.01:5; %Theta range

```

```

at = [];
aU = [];
aL = [];
Et = [];

for a = 0.2:0.003:10
    %If E__L(a) is real it means it's on the EL-line
    if real(E__L(a)) == E__L(a)
        aL = [aL a];
    end
    %If E__U(a) is real it means it's on the EU-line
    if real(E__U(a)) == E__U(a)
        aU = [aU a];
    end
end
end
%The program will now search 'horizontally' for the transition.
for a = min(aU):0.003:max(aU)
    (a-aU(1))/(aU(end)-aU(1))*100 %Progress counter

    for E = min(E__U(aU)):0.001:max(E__U(aU))
        f1 = f(tv, a, E);

        %Finds the first minima of the energy.
        c1 = tv(find(f1(2:end)-f1(1:end-1)>0,1,'first'));

        %Finds the second one.
        c2 = tv(find(f1(2:end)-f1(1:end-1)<0,1,'last'));

        %Checks if a transition happen by looking how far theta jumped
        %compared to the last cycle. Big jump = it changed minima and a
        %transition just took place
        if abs(f(c1, a, E) - f(c2, a, E))<0.001 && abs(c1-c2) > 0.1
            at = [at a];
            Et = [Et E];
            break
        end
    end

end

end

while true
    %The E vs a graph
    figure(1);
    clf
    hold on
    plot(Et, at)
    plot(E__L(aL), aL, 'g--')
    plot(E__U(aU), aU, 'r:')
    text(0.6, 1.86, 'Sm-C_{LT}')
    text(0.6, 1.76, 'Sm-C_{LT}')
end

```

```

text(1, 1.81, 'Sm-C_{HT}')
legend('E_T', 'E_L', 'E_U')
axis([min(E_U(aU))*0.8 max(E_U(aU))*1.2 aU(1)*0.98 aU(end)*1.02])
xlabel('$E$', 'Interpreter', 'LaTeX', 'fontsize', 16)
ylabel('$a$', 'Interpreter', 'LaTeX', 'fontsize', 16)
title('$a$ vs $E(\theta_*)$', 'Interpreter', 'LaTeX', 'fontsize', 16)

[x y] = ginput(1); %Allows us to click in the graph

%The energy density graph
figure(2);
clf
hold on
f1 = f(tv, y, x);
plot(tv, f1)
mm = min(f1);
mt = tv(find(f1 == min(f1)));
plot([-5 5], [mm, mm], 'k--')
plot([mt mt], [-3 3], 'k--')
xlabel('$\theta$', 'Interpreter', 'LaTeX', 'fontsize', 16)
ylabel('$f(\theta)$', 'Interpreter', 'LaTeX', 'fontsize', 16)
axis([-1 3 min(f1)*1.2 0.4])
end

```

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The free energy is defined by the following function. θ is the angle the LC molecules has against the planes between the layers and p is the polarization of the molecule

$$\text{> } f := (\theta, p) \rightarrow \frac{1}{2} r_\theta \theta^2 + \frac{1}{4} u_\theta \theta^4 + \frac{1}{6} v_\theta \theta^6 + \frac{1}{2} r_p p^2 + \frac{1}{4} u_p p^4 + \frac{1}{6} v_p p^6 - E p - e p^2 \theta^2 - \gamma \theta p$$

We can express p in terms of θ by differentiating with respect to θ and solving for the energy minima in terms of p . We find two solutions. We will notice that only the second one will work.

$$\text{> } \text{solve}\left(\frac{\partial}{\partial \theta}(f(\theta, p) = 0), p\right)$$

$$\frac{1}{4} \frac{-\gamma + \sqrt{8 e \theta^6 v_\theta + 8 e \theta^4 u_\theta + 8 e \theta^2 r_\theta + \gamma^2}}{e \theta}, \quad (1)$$

$$-\frac{1}{4} \frac{\gamma + \sqrt{8 e \theta^6 v_\theta + 8 e \theta^4 u_\theta + 8 e \theta^2 r_\theta + \gamma^2}}{e \theta}$$

$$\text{> } p_{\min} := \frac{1}{4} \frac{-\gamma + \sqrt{8 e \theta^6 v_\theta + 8 e \theta^4 u_\theta + 8 e \theta^2 r_\theta + \gamma^2}}{e \theta}$$

To solve for E we first differentiate our free energy with respect to p and again solving for E in the energy minima.

$$\text{> } E := \text{solve}\left(\frac{\partial}{\partial p} f(\theta, p) = 0, E\right)$$

$$E := p^5 v_p - 2 e p \theta^2 + p^3 u_p - \gamma \theta + p r_p \quad (2)$$

Redefining $E(\theta, p)$ as $E(\theta)$ by substituting p with $p_{\min}(\theta)$

$$\text{> } E := \text{subs}(p = p_{\min}, E)$$

$$E := \frac{1}{1024} \frac{v_p \left(-\gamma + \sqrt{8 e \theta^6 v_\theta + 8 e \theta^4 u_\theta + 8 e \theta^2 r_\theta + \gamma^2}\right)^5}{e^5 \theta^5} - \frac{1}{2} \theta \left(-\gamma + \sqrt{8 e \theta^6 v_\theta + 8 e \theta^4 u_\theta + 8 e \theta^2 r_\theta + \gamma^2}\right) + \frac{1}{64} \frac{u_p \left(-\gamma + \sqrt{8 e \theta^6 v_\theta + 8 e \theta^4 u_\theta + 8 e \theta^2 r_\theta + \gamma^2}\right)^3}{e^3 \theta^3} - \gamma \theta + \frac{1}{4} \frac{r_p \left(-\gamma + \sqrt{8 e \theta^6 v_\theta + 8 e \theta^4 u_\theta + 8 e \theta^2 r_\theta + \gamma^2}\right)}{e \theta} \quad (3)$$

We expand E with respect to θ to the fifth order. Giving us E in the following form:

$$E(\theta) = a \theta + b \theta^3 + c \theta^5$$

> $taylor(E, \theta = 0, 11)$

$$\left(-\gamma + \frac{r_p r_\theta}{\gamma} \right) \theta + \left(-\frac{2 e r_\theta}{\gamma} + \frac{u_p r_\theta^3}{\gamma^3} + \frac{1}{4} \frac{r_p \gamma \left(\frac{4 e u_\theta}{\gamma^2} - \frac{8 e^2 r_\theta^2}{\gamma^4} \right)}{e} \right) \theta^3 + \left(\frac{v_p r_\theta^5}{\gamma^5} - \frac{1}{2} \gamma \left(\frac{4 e u_\theta}{\gamma^2} - \frac{8 e^2 r_\theta^2}{\gamma^4} \right) + \frac{3}{4} \frac{u_p r_\theta^2 \left(\frac{4 e u_\theta}{\gamma^2} - \frac{8 e^2 r_\theta^2}{\gamma^4} \right)}{e \gamma} + \frac{1}{4} \frac{r_p \gamma \left(\frac{4 e v_\theta}{\gamma^2} - \frac{16 e^2 r_\theta u_\theta}{\gamma^4} + \frac{32 e^3 r_\theta^3}{\gamma^6} \right)}{e} \right) \theta^5 + o(\theta^7) \quad (4)$$

> $a := r_\theta \rightarrow \left(-\gamma + \frac{1}{4} \frac{r_p \left(-3 \delta + \frac{6 \delta \gamma + 8 e r_\theta}{\gamma} \right)}{e} \right)$

> $b := r_\theta \rightarrow \left(-\frac{2 e r_\theta}{\gamma} + \frac{u_p r_\theta^3}{\gamma^3} + \frac{1}{4} \frac{r_p \gamma \left(\frac{4 e u_\theta}{\gamma^2} - \frac{8 e^2 r_\theta^2}{\gamma^4} \right)}{e} \right)$

> $c := r_\theta$
 $\rightarrow \frac{1}{\gamma^5} \left(-4 e^2 \gamma^2 r_\theta^2 - 8 e^2 r_\theta^3 r_p + 2 e \gamma^4 u_\theta + 4 e \gamma^2 r_\theta r_p u_\theta + 6 e r_\theta^4 u_p - \gamma^4 r_p v_\theta - 3 \gamma^2 r_\theta^2 u_\theta u_p - r_\theta^5 v_p \right)$

> $E := (\theta, a, b, c) \rightarrow a \theta + b \theta^3 + c \theta^5$

We are looking for when $\theta(E)$ has two solutions. We can find it by differentiating E with respect to θ

> $\theta_{\min} := (a, b, c) \rightarrow solve\left(\frac{\partial}{\partial \theta} E(\theta, a, b, c), \theta\right)$

Below we can see four different solutions. Only two of them will work similar to the previous case. By inserting the first solution into $E(\theta, a, b, c)$ we get E_L which is the lower bound where we have two solution. Similarly the third solution gives us E_u the upper bound.

>

> $\theta_{\min}(a, b, c)$

$$\frac{1}{10} \frac{\sqrt{10} \sqrt{c \left(-3 b + \sqrt{-20 a c + 9 b^2} \right)}}{c}, -\frac{1}{10} \frac{\sqrt{10} \sqrt{c \left(-3 b + \sqrt{-20 a c + 9 b^2} \right)}}{c}, \quad (5)$$

$$\frac{1}{10} \frac{\sqrt{-10c(3b + \sqrt{-20ac + 9b^2})}}{c}, -\frac{1}{10} \frac{\sqrt{-10c(3b + \sqrt{-20ac + 9b^2})}}{c}$$

$$> E_L := (a, b, c) \rightarrow \sqrt{-\frac{3b}{10c} - \sqrt{\frac{9}{100} \left(\frac{b}{c}\right)^2 - \frac{a}{5c}}} \left(-\frac{2}{5}b \sqrt{\frac{9}{100} \left(\frac{b}{c}\right)^2 - \frac{a}{5c}} + \frac{4}{5}a - \frac{3}{25} \frac{b^2}{c} \right)$$

$$> E_u := (a, b, c) \rightarrow \sqrt{-\frac{3b}{10c} + \sqrt{\frac{9}{100} \left(\frac{b}{c}\right)^2 - \frac{a}{5c}}} \left(\frac{2}{5}b \sqrt{\frac{9}{100} \left(\frac{b}{c}\right)^2 - \frac{a}{5c}} + \frac{4}{5}a - \frac{3}{25} \frac{b^2}{c} \right)$$

Returning to the expanded version of E. We defined what's in front of the θ as a . We can solve for r_θ and use this to eliminate that parameter in the other terms and instead have a as a changing variable.

$$> r_\theta := a \rightarrow \frac{\gamma(\gamma + a)}{r_p}$$

$$> B := a \rightarrow b(r_\theta(a))$$

$$> B(a)$$

$$-\frac{\frac{2e\gamma^3(\gamma + a)}{r_p} + \frac{2e\gamma^2(\gamma + a)^2}{r_p} - \gamma^2 r_p u_\theta - \frac{\gamma^3(\gamma + a)^3 u_p}{r_p^3}}{\gamma^3} \quad (6)$$

(Using an expansion here just to factor out a)

$$> \text{taylor}(B(a), a=0, 4)$$

$$-\frac{\frac{4e\gamma^4}{r_p} - \gamma^2 r_p u_\theta - \frac{\gamma^6 u_p}{r_p^3}}{\gamma^3} - \frac{\frac{6e\gamma^3}{r_p} - \frac{3\gamma^5 u_p}{r_p^3}}{\gamma^3} a - \frac{\frac{2e\gamma^2}{r_p} - \frac{3\gamma^4 u_p}{r_p^3}}{\gamma^3} a^2 + \frac{u_p}{r_p^3} a^3 \quad (7)$$

$$> b_0 := -\frac{\frac{4e\gamma^4}{r_p} - \gamma^2 r_p u_\theta - \frac{\gamma^6 u_p}{r_p^3}}{\gamma^3}$$

$$> b_1 := -\frac{\frac{6e\gamma^3}{r_p} - \frac{3\gamma^5 u_p}{r_p^3}}{\gamma^3}$$

$$> b_2 := -\frac{\frac{2e\gamma^2}{r_p} - \frac{3\gamma^4 u_p}{r_p^3}}{\gamma^3}$$

$$\left[\begin{array}{l} > b_3 := \frac{u_p}{r_p^3} \end{array} \right.$$

The constant b are now be defined as the function B below

$$\left[\begin{array}{l} > B := (b_0, b_1, b_2, b_3) \rightarrow b_0 + b_1 a + b_2 a^2 + b_3 a^3 \end{array} \right.$$

We do the same thing with c and define it as the function C.

$$\left[\begin{array}{l} > C := a \rightarrow c(r_\theta(a)) \end{array} \right.$$

$$\left[\begin{array}{l} > C(a) \end{array} \right.$$

$$\frac{1}{\gamma^5} \left(-\frac{4e^2 \gamma^4 (\gamma+a)^2}{r_p^2} - \frac{8e^2 \gamma^3 (\gamma+a)^3}{r_p^2} + 2e\gamma^4 u_\theta + 4e\gamma^3 (\gamma+a) u_\theta \right. \tag{8}$$

$$\left. + \frac{6e\gamma^4 (\gamma+a)^4 u_p}{r_p^4} - \gamma^4 r_p v_\theta - \frac{3\gamma^4 (\gamma+a)^2 u_\theta u_p}{r_p^2} - \frac{\gamma^5 (\gamma+a)^5 v_p}{r_p^5} \right)$$

$$\left[\begin{array}{l} > \text{taylor}(C(a), a=0, 6) \end{array} \right.$$

$$\frac{-\frac{12e^2 \gamma^6}{r_p^2} + 6e\gamma^4 u_\theta + \frac{6e\gamma^8 u_p}{r_p^4} - \gamma^4 r_p v_\theta - \frac{3\gamma^6 u_\theta u_p}{r_p^2} - \frac{\gamma^{10} v_p}{r_p^5}}{\gamma^5} \tag{9}$$

$$+ \frac{-\frac{32e^2 \gamma^5}{r_p^2} + 4e\gamma^3 u_\theta + \frac{24e\gamma^7 u_p}{r_p^4} - \frac{6\gamma^5 u_\theta u_p}{r_p^2} - \frac{5\gamma^9 v_p}{r_p^5}}{\gamma^5} a$$

$$+ \frac{-\frac{28e^2 \gamma^4}{r_p^2} + \frac{36e\gamma^6 u_p}{r_p^4} - \frac{3\gamma^4 u_\theta u_p}{r_p^2} - \frac{10\gamma^8 v_p}{r_p^5}}{\gamma^5} a^2$$

$$+ \frac{-\frac{8e^2 \gamma^3}{r_p^2} + \frac{24e\gamma^5 u_p}{r_p^4} - \frac{10\gamma^7 v_p}{r_p^5}}{\gamma^5} a^3 + \frac{\frac{6e\gamma^4 u_p}{r_p^4} - \frac{5\gamma^6 v_p}{r_p^5}}{\gamma^5} a^4 - \frac{v_p}{r_p^5} a^5$$

$$\left[\begin{array}{l} > c_0 := \frac{-\frac{12e^2 \gamma^6}{r_p^2} + 6e\gamma^4 u_\theta + \frac{6e\gamma^8 u_p}{r_p^4} - \gamma^4 r_p v_\theta - \frac{3\gamma^6 u_\theta u_p}{r_p^2} - \frac{\gamma^{10} v_p}{r_p^5}}{\gamma^5} \end{array} \right.$$

$$\left[\begin{array}{l} > c_1 := \frac{-\frac{32e^2 \gamma^5}{r_p^2} + 4e\gamma^3 u_\theta + \frac{24e\gamma^7 u_p}{r_p^4} - \frac{6\gamma^5 u_\theta u_p}{r_p^2} - \frac{5\gamma^9 v_p}{r_p^5}}{\gamma^5} \end{array} \right.$$

$$> c_2 := \frac{-\frac{28 e^2 \gamma^4}{r_p^2} + \frac{36 e \gamma^6 u_p}{r_p^4} - \frac{3 \gamma^4 u_\theta u_p}{r_p^2} - \frac{10 \gamma^8 v_p}{r_p^5}}{\gamma^5}$$

$$> c_3 := \frac{-\frac{8 e^2 \gamma^3}{r_p^2} + \frac{24 e \gamma^5 u_p}{r_p^4} - \frac{10 \gamma^7 v_p}{r_p^5}}{\gamma^5}$$

$$> c_4 := \frac{\frac{6 e \gamma^4 u_p}{r_p^4} - \frac{5 \gamma^6 v_p}{r_p^5}}{\gamma^5}$$

$$> c_5 := -\frac{v_p}{r_p^5}$$

$$> C := (c_0, c_1, c_2, c_3, c_4, c_5) \rightarrow c_0 + c_1 a + c_2 a^2 + c_3 a^3 + c_4 a^4 + c_5 a^5$$

Looking at θ_{\min} we notice that what's under the root signs must be positive for the result to be real. Specifically what's under the second root sign is worth looking at. We define what's under there as the function R .

$$> R := B(b_0, b_1, b_2, b_3)^2 - \frac{20}{9} a C(c_0, c_1, c_2, c_3, c_4, c_5)$$

$$> \text{taylor}(R, a=0, 7)$$

$$b_0^2 + \left(2 b_0 b_1 - \frac{20}{9} c_0\right) a + \left(2 b_0 b_2 + b_1^2 - \frac{20}{9} c_1\right) a^2 + \left(2 b_0 b_3 + 2 b_1 b_2 - \frac{20}{9} c_2\right) a^3 + \left(2 b_1 b_3 + b_2^2 - \frac{20}{9} c_3\right) a^4 + \left(2 b_2 b_3 - \frac{20}{9} c_4\right) a^5 + \left(b_3^2 - \frac{20}{9} c_5\right) a^6 \quad (10)$$

$$\begin{bmatrix} b_0 = b_0 \\ b_1 = b_1 \\ b_2 = b_2 \\ b_3 = b_3 \\ c_0 = c_0 \\ c_1 = c_1 \\ c_2 = c_2 \\ c_3 = c_3 \\ c_4 = c_4 \\ c_5 = c_5 \end{bmatrix}$$

>

$$b_0 = -\frac{\frac{4e\gamma^4}{r_p} - \gamma^2 r_p u_\theta - \frac{\gamma^6 u_p}{r_p^3}}{\gamma^3}$$

$$b_1 = -\frac{\frac{6e\gamma^3}{r_p} - \frac{3\gamma^5 u_p}{r_p^3}}{\gamma^3}$$

$$b_2 = -\frac{\frac{2e\gamma^2}{r_p} - \frac{3\gamma^4 u_p}{r_p^3}}{\gamma^3}$$

$$b_3 = \frac{u_p}{r_p^3}$$

$$c_0 = \frac{-\frac{12e^2\gamma^6}{r_p^2} + 6e\gamma^4 u_\theta + \frac{6e\gamma^8 u_p}{r_p^4} - \gamma^4 r_p v_\theta - \frac{3\gamma^6 u_\theta u_p}{r_p^2} - \frac{\gamma^{10} v_p}{r_p^5}}{\gamma^5}$$

$$c_1 = \frac{-\frac{32e^2\gamma^5}{r_p^2} + 4e\gamma^3 u_\theta + \frac{24e\gamma^7 u_p}{r_p^4} - \frac{6\gamma^5 u_\theta u_p}{r_p^2} - \frac{5\gamma^9 v_p}{r_p^5}}{\gamma^5}$$

$$c_2 = \frac{-\frac{28e^2\gamma^4}{r_p^2} + \frac{36e\gamma^6 u_p}{r_p^4} - \frac{3\gamma^4 u_\theta u_p}{r_p^2} - \frac{10\gamma^8 v_p}{r_p^5}}{\gamma^5}$$

$$c_3 = \frac{-\frac{8e^2\gamma^3}{r_p^2} + \frac{24e\gamma^5 u_p}{r_p^4} - \frac{10\gamma^7 v_p}{r_p^5}}{\gamma^5}$$

$$c_4 = \frac{\frac{6e\gamma^4 u_p}{r_p^4} - \frac{5\gamma^6 v_p}{r_p^5}}{\gamma^5}$$

$$c_5 = -\frac{v_p}{r_p^5}$$

(11)

We have now found all requirements for $\theta(E)$ to have two solutions in certain ranges.

$$B(a) < 0$$

$$R(a) > 0$$

This must happen in a common region of a .

In addition to this, $C(a)$ must be greater than 0 when $a > 0$

From this it follows that:

$$b_0 > 0$$

$$c_0 > 0$$

$$c_5 > 0$$

We can use this to simplify our equations making it easier for us to find values that fulfil all our requirements

>

$$Su_p := \text{solve}(b3 = b_3, u_p)$$

$$Su_p := b_3 r_p^3 \quad (12)$$

$$b_0 := \text{subs}(u_p = Su_p, b_0)$$

$$b_0 := -\frac{\frac{4 e \gamma^4}{r_p} - \gamma^2 r_p u_\theta - \gamma^6 b_3}{\gamma^3} \quad (13)$$

$$Su_\theta := \text{solve}(b_0 = b_\theta, u_\theta)$$

$$Su_\theta := -\frac{\gamma(-b_0 r_p^3 - 4 e \gamma r_p^2 + \gamma^3 u_p)}{r_p^4} \quad (14)$$

$$c_0 := \text{expand}(\text{subs}([u_\theta = Su_\theta, u_p = Su_p], c_0))$$

$$c_0 := \frac{12 \gamma e^2}{r_p^2} + \frac{6 e b_0}{r_p} - \frac{6 \gamma^3 e u_p}{r_p^4} - \frac{6 \gamma^3 e b_3}{r_p} - \frac{r_p v_\theta}{\gamma} - 3 \gamma^2 b_3 b_0 + \frac{3 \gamma^5 b_3 u_p}{r_p^3} - \frac{\gamma^5 v_p}{r_p^5} \quad (15)$$

>

$$Sv_\theta := \text{solve}(c_0 = c_\theta, v_\theta)$$

$$Sv_\theta := -\frac{c_0 \gamma r_p^5 + 12 e^2 \gamma^2 r_p^3 - 6 e \gamma^4 r_p u_p - 6 e r_p^5 u_\theta + \gamma^6 v_p + 3 \gamma^2 r_p^3 u_p u_\theta}{r_p^6} \quad (16)$$

>

$$Sv_p := \text{solve}(c_5 = c_5, v_p)$$

$$Sv_p := -c_5 r_p^5 \quad (17)$$

$$Sv_\theta := \text{subs}(v_p = Sv_p, Sv_\theta)$$

$$Sv_\theta := -\frac{-c_5 \gamma^6 r_p^5 + c_0 \gamma r_p^5 + 12 e^2 \gamma^2 r_p^3 - 6 e \gamma^4 r_p u_p - 6 e r_p^5 u_\theta + 3 \gamma^2 r_p^3 u_p u_\theta}{r_p^6} \quad (18)$$

$$S := [u_\theta = Su_\theta, u_p = Su_p, v_\theta = Sv_\theta, v_p = Sv_p]$$

$$S := \left[u_\theta = -\frac{\gamma(-b_0 r_p^3 - 4e\gamma r_p^2 + \gamma^3 u_p)}{r_p^4}, u_p = b_3 r_p^3, v_\theta = \right. \\ \left. -\frac{-c_5 \gamma^6 r_p^5 + c_0 \gamma r_p^5 + 12e^2 \gamma^2 r_p^3 - 6e\gamma^4 r_p u_p - 6e r_p^5 u_\theta + 3\gamma^2 r_p^3 u_p u_\theta}{r_p^6}, v_p = -c_5 r_p^5 \right] \quad (19)$$

> $b_1 := \text{subs}(S, b_1)$

> $b_2 := \text{subs}(S, b_2)$

> $c_1 := \text{subs}(S, c_1)$

> $c_2 := \text{subs}(S, c_2)$

> $c_3 := \text{subs}(S, c_3)$

> $c_4 := \text{subs}(S, c_4)$

>
$$\left[\begin{array}{l} b_0 = b_0 \\ b_1 = b_1 \\ b_2 = b_2 \\ b_3 = b_3 \\ c_0 = c_0 \\ c_1 = \text{expand}(c_1) \\ c_2 = \text{expand}(c_2) \\ c_3 = \text{expand}(c_3) \\ c_4 = c_4 \\ c_5 = c_5 \end{array} \right]$$

$$\begin{aligned}
b_0 &= b0 \\
b_1 &= -\frac{\frac{6e\gamma^3}{r_p} - 3\gamma^5 b3}{\gamma^3} \\
b_2 &= -\frac{\frac{2e\gamma^2}{r_p} - 3\gamma^4 b3}{\gamma^3} \\
b_3 &= b3 \\
c_0 &= c0 \\
c_1 &= -\frac{16e^2}{r_p^2} + \frac{4eb0}{\gamma r_p} - \frac{4\gamma^2 e u_p}{r_p^4} - 6\gamma b3 b0 + \frac{6\gamma^4 b3 u_p}{r_p^3} + 5\gamma^4 c5 \\
c_2 &= -\frac{28e^2}{\gamma r_p^2} + \frac{24\gamma e b3}{r_p} - 3b3 b0 + \frac{3\gamma^3 b3 u_p}{r_p^3} + 10\gamma^3 c5 \\
c_3 &= -\frac{8e^2}{\gamma^2 r_p^2} + \frac{24eb3}{r_p} + 10\gamma^2 c5 \\
c_4 &= \frac{\frac{6e\gamma^4 b3}{r_p} + 5\gamma^6 c5}{\gamma^5} \\
c_5 &= c5
\end{aligned}
\tag{20}$$

To solve for the different parameter values that would fulfil all these requirements is difficult. But by using MATLAB to bruteforce a solution shows us it is possible.

