Some examples of calculus of variations of discontinuous functions and their implications

Shengnan Huang

School of Physics, Georgia Institute of Technology,
837 State Street, Atlanta, GA 30332

November 25, 2018

Abstract

We consider functions defined on $[0, L]$ with special jump discontinuities, and discuss two different methods of doing calculus of variations. One method is to solve the boundary value problem in each sub-region divided by the discontinuities, and the other method is to use Fourier series on the whole region. We argue that the second method, though has an energy divergence problem, can lead to a unified view of similar examples and may provide a way of studying nematic defects.

1 Examples

1.1 Example 1

Consider a function $f : U \to \mathbb{R}$, where $U = [0, L_1) \cup (L_1, L]$ with L_1 being a variable, and an energy functional

$$F[f(x), f'(x)] = \int_U \left(\frac{\mathrm{d}f}{\mathrm{d}x}\right)^2 \mathrm{d}x. \tag{1}$$

The outer boundary conditions are

$$f(0) = f(L) = 0. \tag{2}$$

The inner boundary conditions are

$$f(L_1^-) = -f(L_1^+) = -a, \tag{3}$$

where L, a are fixed parameters. The question is: what is the ground state when L_1 varies?

This is a special example of calculus of variations where the function space consists of functions which are smooth except on a subset of measure zero. An illustration of the steps of doing this calculus of variations is the following:

Let us start with the action

$$F[f(x), f'(x)] = \int_U \mathrm{d}x\ \mathcal{F}(f(x), f'(x)), \tag{4}$$

where $f(x)$ are those generalized functions satisfying the boundary conditions Eqs. (2) and (3). Then let $f_b(x), f_c(x)$ denote the functions $f(x)$ with discontinuities being at $L_1 = b, c$ [i.e., $f_b(b^-) = -f_b(b^+) = -a$, $f_c(c^-) = -f_c(c^+) = -a$], and let $\delta f_b(x), \delta f_c(x)$ denote the variations on $f_b(x), f_c(x)$ with $\delta f_b(b^-) = \delta f_b(b^+) = 0$, $\delta f_c(c^-) = \delta f_c(c^+) = 0$. Assume $\delta f_b(x), \delta f_c(x)$ are small, and $|c - b| \ll 1$. Then,

$$0 = F[f_c + \delta f_c] - F[f_b] = (F[f_c + \delta f_c] - F[f_c]) + (F[f_c] - F[f_b]), \tag{5}$$

which is

$$\int_U \Big(\frac{\partial \mathcal{F}}{\partial f_c} - \frac{\mathrm{d}}{\mathrm{d}x}\Big(\frac{\partial \mathcal{F}}{\partial f_c'}\Big)\Big)\delta f_c = F[f_b] - F[f_c] = F(L_1 = b) - F(L_1 = c) = \frac{\mathrm{d}F}{\mathrm{d}L_1}\Big|_{L_1=c} \cdot (b-c). \tag{6}$$

Note that we do not consider $F[f_c + \delta f_b]$ because $f_c + \delta f_b$ does not satisfy the boundary conditions thus it is not in the function space we consider. Because b, c, and δf_c are independent, so we have

$$\frac{\partial \mathcal{F}}{\partial f} - \frac{\mathrm{d}}{\mathrm{d}x}\Big(\frac{\partial \mathcal{F}}{\partial f'}\Big) = 0, \tag{7}$$

$$\frac{\mathrm{d}F}{\mathrm{d}L_1} = 0. \tag{8}$$

Equations (5)-(8) implies that the small change of the functional F around a equilibrium state can be decomposed into two parts: (1) the small change due to the change of the function f with the location of discontinuity fixed, and (2) the small change due to the change of the locations of discontinuities.

Now let us write down the second functional derivatives

$$\begin{aligned} F[f_c + \delta f_c] - F[f_b] &= (F[f_c + \delta f_c] - F[f_c]) + (F[f_c] - F[f_b]) \\ &= 0 + \int \mathrm{d}x_1 \int \mathrm{d}x_2 \ \frac{\delta^2 \mathcal{F}}{\delta f_c(x_1)\delta f_c(x_2)} \delta f_c(x_1)\delta f_c(x_2) + \frac{1}{2}\frac{\mathrm{d}^2 F}{\mathrm{d}L_1^2}\Big|_{L_1=c} \cdot (b-c)^2. \end{aligned} \tag{9}$$

To make sure f is a local energy minimizer, we require both

$$\frac{\delta^2 \mathcal{F}}{\delta f(x_1)\delta f(x_2)} \geq 0, \tag{10}$$

and

$$\frac{\mathrm{d}^2 F}{\mathrm{d}L_1^2} \geq 0. \tag{11}$$

Now following the above procedure, it is easy to find the ground state of Example 1. We start with the Euler-Lagrange equation

$$\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} = 0, \tag{12}$$

which is satisfied on $[0, L_1) \cup (L_1, L]$. Then we obtain its solution

$$f(x) = \begin{cases} -\frac{a}{L_1}x, x \in [0, L_1), \\ \\ -\frac{a}{L-L_1}x + \frac{L}{L-L_1}a, x \in (L_1, L]. \end{cases} \tag{13}$$

Substitute Eq. (13) into Eq. (1), and we have the following energy landscape

$$F(L_1) = \frac{a^2}{L_1} + \frac{a^2}{L - L_1}, \tag{14}$$

and the ground state is $L_1 = L/2$.

1.2 Example 2

Consider a similar but slightly more difficult example with the energy functional

$$F[f(x), f'(x)] = \int_U \Big[\Big(\frac{\mathrm{d}f}{\mathrm{d}x}\Big)^2 + A^2 f^2\Big]\mathrm{d}x, \tag{15}$$

where f satisfies the same boundary conditions as Eqs. (2) and (3).

Similarly, the Euler-Lagrange equation is

$$\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} - A^2 f = 0, \tag{16}$$

and its solution is

$$f(x) = \begin{cases} -\frac{a}{e^{AL_1} - e^{-AL_1}} e^{Ax} + \frac{a}{e^{AL_1} - e^{-AL_1}} e^{-Ax}, x \in [0, L_1), \\ \frac{a}{e^{AL_1} - e^{2AL - AL_1}} e^{Ax} - \frac{a}{e^{-2AL + AL_1} - e^{-AL_1}} e^{-Ax}, x \in (L_1, L]. \end{cases} \tag{17}$$

Substitute Eq. (17) into Eq. (16), and we have the following energy landscape

$$F(L_1) = a^2 A \cdot \frac{e^{AL_1} + e^{-AL_1}}{e^{AL_1} - e^{-AL_1}} + a^2 A \cdot \frac{e^{2AL - AL_1} + e^{AL_1}}{e^{2AL - AL_1} - e^{AL_1}} \tag{18}$$

and the ground state is still $L_1 = L/2$.

Compared with Example 1, Example 2 has only a slight modification, and we find that the ground state is unchanged but the calculation is much more involved. It is expected that for higher dimensions, more complicated PDEs and boundaries, this method, let us call it Method (a), may be sometimes impossible to execute. The reason is that it requires solving a boundary value problem in each sub-region. Since our goal is focused on the states characterized by the locations of the inner boundaries (discontinuities), there should be a method that is able to extract the information of inner boundaries without dwelling on the exact forms of the solutions. To work in this direction, we treat all the sub-regions together as a whole, using Fourier series as the "glue". Let us call it Method (b).

1.3 Solving Example 1 by Method (b)

We write f as Fourier series of sine functions

$$f(x) = \sum_{k=1}^{\infty} b_k \sin \frac{k\pi x}{L}, \tag{19}$$

where b_k is unknown. Then we write its first derivative as

$$\frac{\mathrm{d}f}{\mathrm{d}x} = \sum_{k=1}^{\infty} \frac{k\pi b_k}{L} \cos \frac{k\pi x}{L}. \tag{20}$$

When written in terms of Fourier series, $f(x)$ and $f'(x)$ are assigned certain values at the discontinuous point $x = L_1$. Here, the energy functional is still denoted by $F[f(x), f'(x)]$ while we should keep in mind that $f(x)$ and $f'(x)$ are expressed as Eqs. (19) and (20).

Now we want to construct an energy function of which the small change only includes the change of the location of the discontinuity. We start by deriving the expression for b_k:

On $[0, L_1)$, from Eq. (12), we have

$$\begin{aligned} 0 &= \int_0^{L_1^-} \frac{\mathrm{d}^2 f}{\mathrm{d}x^2} \sin \frac{k\pi x}{L} \mathrm{d}x = \int_0^{L_1^-} \sin \frac{k\pi x}{L} \mathrm{d}\Big(\frac{\mathrm{d}f}{\mathrm{d}x}\Big) \\ &= \sin \frac{k\pi L_1}{L} \cdot \frac{\mathrm{d}f}{\mathrm{d}x}\Big|_{L_1} + \frac{k\pi a}{L} \cos \frac{k\pi L_1}{L} - \Big(\frac{k\pi}{L}\Big)^2 \int_0^{L_1^-} f \sin \frac{k\pi x}{L} \mathrm{d}x. \end{aligned} \tag{21}$$

Therefore,

$$\int_0^{L_1} f \sin \frac{k\pi x}{L} \mathrm{d}x = \frac{aL}{k\pi} \cos \frac{k\pi L_1}{L} + \Big(\frac{L}{k\pi}\Big)^2 \sin \frac{k\pi L_1}{L} \cdot \frac{\mathrm{d}f}{\mathrm{d}x}\Big|_{L_1^-}. \tag{22}$$

Similarly, on $(L_1, L]$

$$\int_{L_1^+}^{L} f \sin\frac{k\pi x}{L}\mathrm{d}x = \frac{aL}{k\pi}\cos\frac{k\pi L_1}{L} - \Big(\frac{L}{k\pi}\Big)^2 \sin\frac{k\pi L_1}{L}\cdot\frac{\mathrm{d}f}{\mathrm{d}x}\Big|_{L_1^+}. \tag{23}$$

Therefore,

$$\begin{aligned} b_k &= \frac{2}{L}\int_0^L f\sin\frac{k\pi x}{L}\mathrm{d}x = \frac{2}{L}\Big(\int_0^{L_1^-} f\sin\frac{k\pi x}{L}\mathrm{d}x + \int_{L_1^+}^{L} f\sin\frac{k\pi x}{L}\mathrm{d}x\Big) \\ &= \frac{4a}{k\pi}\cos\frac{k\pi L_1}{L} + \frac{2L}{(k\pi)^2}B\sin\frac{k\pi L_1}{L}, \end{aligned} \tag{24}$$

where

$$B = \frac{\mathrm{d}f}{\mathrm{d}x}\Big|_{L_1^+} - \frac{\mathrm{d}f}{\mathrm{d}x}\Big|_{L_1^-}.$$

Note that Eq. (24) takes advantage of the fact that f is bounded and the discontinuity is on a set with measure zero. To determine the only unknown B in the expression for b_k, we use Dirichlet conditions, specifically, the fact that f, when written in terms of Fourier series as Eq. (19), is zero at the discontinuity. Therefore, we have

$$\sum_{k=1}^{\infty}\Big(\frac{4a}{k\pi}\cos\frac{k\pi L_1}{L} + \frac{2L}{(k\pi)^2}B\sin\frac{k\pi L_1}{L}\Big)\sin\frac{k\pi L_1}{L} = 0, \tag{25}$$

and it gives

$$B = a\Big(\frac{1}{L-L_1} - \frac{1}{L_1}\Big). \tag{26}$$

Substitute Eq. (26) into Eq. (24) and then substitute Eq. (24) into Eq. (19) and (20), we have

$$f(x) = f_1(x) + f_2(x), \tag{27}$$

where

$$f_1(x) = \sum_{k=1}^{\infty}\frac{4a}{k\pi}\cos\frac{k\pi L_1}{L}\sin\frac{k\pi x}{L}, \tag{28}$$

$$f_2(x) = \sum_{k=1}^{\infty}\frac{2L\cdot B}{(k\pi)^2}\sin\frac{k\pi L_1}{L}\sin\frac{k\pi x}{L} = \sum_{k=1}^{\infty}\frac{2aL}{(k\pi)^2}\Big(\frac{1}{L-L_1} - \frac{1}{L_1}\Big)\sin\frac{k\pi L_1}{L}\sin\frac{k\pi x}{L}; \tag{29}$$

and

$$\begin{aligned} \frac{\mathrm{d}f}{\mathrm{d}x} &= \sum_{k=1}^{\infty}\Big[4a\cos\frac{k\pi L_1}{L} + \frac{2L\cdot B}{k\pi}\sin\frac{k\pi L_1}{L}\Big]\cdot\frac{1}{L}\cos\frac{k\pi x}{L} \\ &= \sum_{k=1}^{\infty}\Big[4a\cos\frac{k\pi L_1}{L} + \frac{2aL}{k\pi}\Big(\frac{1}{L-L_1} - \frac{1}{L_1}\Big)\sin\frac{k\pi L_1}{L}\Big]\cdot\frac{1}{L}\cos\frac{k\pi x}{L}. \end{aligned} \tag{30}$$

Then in order to get the energy function, we substitute Eqs. (27) and (30) into

$$F[f(x), f'(x)] = \int_0^L \Big(\frac{\mathrm{d}f}{\mathrm{d}x}\Big)^2\mathrm{d}x. \tag{31}$$

Knowing that Eq. (30) can be highly oscillated, therefore in order to suppress the possible high oscillation of the resulting energy function $F(L_1)$, we require $f'(L_1)$ to be differentiable with respect to L_1. This is due to our observation that this condition makes sure the "core structures" at different $x = L_1$ for fixed N terms truncation are almost the same, which implies that the free energy of the core will not oscillate rapidly as L_1 changes. Starting from here, a more explicit condition is derived as follows:

Truncate Eq. (30) to the Nth term and evaluate it at $x = L_1$, we have

$$\begin{aligned}\frac{\mathrm{d}f_N}{\mathrm{d}x}\Big|_{x\,=L_1} &= \sum_{k=1}^{N}\Big[4a\cos\frac{k\pi L_1}{L} + \frac{2aL}{k\pi}\Big(\frac{1}{L-L_1} - \frac{1}{L_1}\Big)\sin\frac{k\pi L_1}{L}\Big]\cdot\frac{1}{L}\cos\Big(\frac{k\pi L_1}{L}\Big) \\ &= \frac{a}{L}\cdot\frac{\cos\frac{2N\pi L_1}{L} - \cos\frac{2(N+1)\pi L_1}{L}}{1-\cos\frac{2\pi L_1}{L}} + \frac{a}{L}\cdot(2N-1) - \frac{a}{2L}\cdot\frac{(L-2L_1)^2}{L_1(L-L_1)},\end{aligned} \tag{32}$$

as $N \to \infty$. To make sure Eq. (32) is differentiable, we apply the following condition

$$N\cdot\frac{L_1}{L} \in \mathbb{Z}. \tag{33}$$

That implies, when N is fixed, we can use the energy functional $F[f_N(x), f_N'(x)]$ for only finite number of states characterized by different values of L_1, and only when $N \to \infty$ can this functional be effective for all the states. Now we show that (33) is both a necessary and sufficient condition for $f'(L_1)$ being differentiable:

Proof. Part I: Prove (33) is a necessary condition.

If L_1/L is a rational number, then obviously we can choose an integer N_1 that satisfies (33). For many different rational values of L_1/L, we can choose N to be the least common multiple of all the N_1s. If L_1/L is an irrational number, then for any arbitrary small number δ_1, there exists an integer N_1, such that

$$N_1\cdot\frac{L_1}{L} - \delta_1 \in \mathbb{Z}. \tag{34}$$

For many different irrational values of L_1/L, we can choose N to be the least common multiple of all the N_1s, and each δ_1 to be replace by δ/N, where δ is arbitrarily small. Therefore, (33) can be satisfied by L_1/L being any real number. Then we substitute Eq. (32) into Eq. (32), and the resulting $f'(L_1)$ is differentiable.

Part II: Prove (33) is a sufficient condition.

Suppose

$$N\cdot\frac{L_1}{L} - m \in \mathbb{Z}, \tag{35}$$

where m is fixed for all different values of L_1/L, and $0 < m < 1$. If m is a rational number, then we write m as $m = m_1/m_2$, where m_1, $m_2 \in \mathbb{Z}$ and $m_2 \nmid m_1$. Since N is an integer, we have the following condition

$$\frac{m_1}{m_2}\cdot\frac{L}{L_1} \in \mathbb{Z}. \tag{36}$$

which cannot be satisfied by some values of L_1/L. The reason is similar if m is an irrational number. Now suppose one value of L_1/L is not satisfied by (36), and $N\cdot\frac{L_1}{L} - n \in \mathbb{Z}$ (where $n \neq m$). Then $\frac{L_1}{L} + \frac{m-n}{N}$ which is very close to L_1/L satisfies (36), therefore $f'(L_1)$ is not differentiable at this value of L_1/L. □

After we substitute Eqs. (27) and (30) into Eq. (31), Equation (31) becomes

$$F(L_1) = \sum_{k=1}^{\infty}\frac{(b_k k\pi)^2}{2L} = F_1(L_1) + F_2(L_1) + F_3(L_1), \tag{37}$$

where

$$F_1(L_1) = \frac{1}{2L}\cdot\sum_{k=1}^{\infty}\Big(4a\cos\frac{k\pi L_1}{L}\Big)^2, \tag{38}$$

$$F_2(L_1) = \frac{1}{2L} \cdot \sum_{k=1}^{\infty} \Big(\frac{2L \cdot B}{k\pi} \sin \frac{k\pi L_1}{L}\Big)^2 = \frac{1}{2L} \cdot \sum_{k=1}^{\infty} \Big[\frac{2aL}{k\pi}\Big(\frac{1}{L-L_1} - \frac{1}{L_1}\Big) \sin \frac{k\pi L_1}{L}\Big]^2, \tag{39}$$

$$\begin{aligned} F_3(L_1) &= \frac{1}{L} \cdot \sum_{k=1}^{\infty} \Big(4a \cos \frac{k\pi L_1}{L}\Big) \cdot \Big(\frac{2L \cdot B}{k\pi} \sin \frac{k\pi L_1}{L}\Big) \\ &= \frac{1}{L} \cdot \sum_{k=1}^{\infty} \Big(4a \cos \frac{k\pi L_1}{L}\Big) \cdot \Big[\frac{2aL}{k\pi}\Big(\frac{1}{L-L_1} - \frac{1}{L_1}\Big) \sin \frac{k\pi L_1}{L}\Big]. \end{aligned} \tag{40}$$

F_1 is insanely divergent, while interestingly for F_2 we have

$$F_2(L_1) = \frac{1}{2L} \cdot \sum_{k=1}^{\infty} \Big[\frac{2aL}{k\pi}\Big(\frac{1}{L-L_1} - \frac{1}{L_1}\Big) \sin \frac{k\pi L_1}{L}\Big]^2 = \frac{a^2}{L_1} + \frac{a^2}{L-L_1} - \frac{4a^2}{L}. \tag{41}$$

We can see that Eqs. (41) and (14) are equally effective in determining the ground state. Now we should figure out why we should cancel out $F_1(L_1)$ and $F_3(L_1)$.

Consider the following energy functional

$$F(y, L_1) = \int_0^y \Big(\frac{\mathrm{d}f}{\mathrm{d}x}\Big)^2 \mathrm{d}x = F_1(y, L_1) + F_2(y, L_1) + F_3(y, L_1), \tag{42}$$

where $F(L, L_1) = F(L_1)$, $F_1(L, L_1) = F_1(L_1)$, $F_2(L, L_1) = F_2(L_1)$, and $F_3(L, L_1) = F_3(L_1)$. After tedious calculations, we have

$$\begin{aligned} F_1(y, L_1) = {} & \frac{4a^2}{L^2} \cdot \lim_{N\to\infty} \sum_{k=1}^{N} \Big(y + y \cdot \cos \frac{2k\pi L_1}{L}\Big) \\ & + \frac{4a^2}{L^2} \cdot \lim_{N\to\infty} \sum_{k_1,k_2=1,k_1\neq k_2,}^{N} \Big[\frac{L}{(k_1-k_2)\pi} \cos \frac{(k_1-k_2)\pi L_1}{L} \sin \frac{(k_1-k_2)\pi y}{L} \\ & + \frac{L}{(k_1-k_2)\pi} \cos \frac{(k_1+k_2)\pi L_1}{L} \sin \frac{(k_1-k_2)\pi y}{L}\Big] \\ & + \frac{4a^2}{L^2} \cdot \lim_{N\to\infty} \sum_{k_1,k_2=1}^{N} \Big[\frac{L}{(k_1+k_2)\pi} \cos \frac{(k_1-k_2)\pi L_1}{L} \sin \frac{(k_1+k_2)\pi y}{L} \\ & + \frac{L}{(k_1+k_2)\pi} \cos \frac{(k_1+k_2)\pi L_1}{L} \sin \frac{(k_1+k_2)\pi y}{L}\Big] \\ = {} & \frac{2a^2 y}{L^2}\Big(\frac{\cos \frac{2N\pi L_1}{L} - \cos \frac{2(N+1)\pi L_1}{L}}{1 - \cos \frac{2\pi L_1}{L}} - 1\Big) \\ & - \frac{2a^2}{\pi L} \cdot \frac{\sin \frac{\pi y}{L}}{\cos \frac{\pi L_1}{L} - \cos \frac{\pi y}{L}} + \frac{a^2}{\pi L} \cdot \frac{\cos \frac{(2N+1)\pi L_1}{L}}{\sin \frac{\pi L_1}{L}} \ln \left(\frac{1 - \cos \frac{\pi(y-L_1)}{L}}{1 - \cos \frac{\pi(y+L_1)}{L}}\right) + \frac{4a^2 y}{L^2} \\ & + \begin{cases} 0 + \frac{2a^2 y}{L^2}\Big(1 - \frac{\sin \frac{(2N+1)\pi L_1}{L}}{\sin \frac{\pi L_1}{L}}\Big), & \text{if } 0 < y < L_1 \\ \frac{4(N-1)a^2}{L} + \frac{2a^2(L-y)}{L^2}\Big(-1 + \frac{\sin \frac{(2N+1)\pi L_1}{L}}{\sin \frac{\pi L_1}{L}}\Big), & \text{if } L_1 < y < L \end{cases} \\ = {} & -\frac{2a^2}{\pi L} \cdot \frac{\sin \frac{\pi y}{L}}{\cos \frac{\pi L_1}{L} - \cos \frac{\pi y}{L}} + \frac{a^2}{\pi L} \\ & \cdot \frac{\cos \frac{\pi L_1}{L}}{\sin \frac{\pi L_1}{L}} \ln \left(\frac{1 - \cos \frac{\pi(y-L_1)}{L}}{1 - \cos \frac{\pi(y+L_1)}{L}}\right) + \frac{4a^2 y}{L^2} + \begin{cases} 0, & \text{if } 0 < y < L_1 \\ \frac{4(N-1)a^2}{L}, & \text{if } L_1 < y < L \end{cases} \end{aligned} \tag{43}$$

and its density profile

$$\begin{aligned}\mathcal{F}_1(y,L_1) = \frac{4a^2}{L^2} + \frac{a^2}{2L^2}\Bigg(&\csc^2\frac{\pi(y-L_1)}{2L} + \cos\frac{\pi(y-3L_1)}{2L} - \cos\frac{\pi(y+L_1)}{2L} \\ &+ \cot\frac{\pi L_1}{L}\csc^2\frac{\pi(y-L_1)}{2L}\csc\frac{\pi(y+L_1)}{2L} + \csc^2\frac{\pi(y+L_1)}{2L}\Bigg).\end{aligned} \tag{44}$$

From Eq. (43), we can see that condition (33) guarantees that $F_1(L_1)$ is a constant even though it is infinite. From the energy density profile Eq. (44), we can see $F_1(L_1)$ consists of three parts: (a) the fictitious core free energy caused by the discontinuity, (b) the fictitious fluctuation energy caused by the large oscillations near the discontinuity (i.e., Gibbs phenomenon), and (c) the part of energy which is not the core or fluctuation energy, i.e., $4a^2/L$.

Now let us have a more detailed comparison between Method (a) and (b) in solving Example 1:

For clarity, let us denote the function and energy in Method (a) by g and G respectively instead of f and F, while keeping the notations in Method (b) unchanged. We observe that when the location of the discontinuity is fixed at $x = L_1$, the only difference between g and f is that f has an (almost) perpendicular line at $x = L_1$ and large oscillations near it. Let η and ξ denote these two effects respectively, thus the above description can be summarized as

$$f = g + \eta + \xi. \tag{45}$$

According to Eqs. (27)-(29), g can be decomposed as

$$g = (g - f_2) + f_2. \tag{46}$$

Compare the energy functions Eqs. (14), (37)-(41) and (43), we have the following observations:

(a) $g = (g - f_2) + f_2$ contributes to the real energy $G(L_1)$, where $g - f_2$ contributes to the part which is independent of L_1 [i.e., $4a^2/L$];

(b) $(g - f_2) + \eta + \xi$ contributes to the energy $F_1(L_1)$ which is infinitely large but also independent of L_1 (and we call it the background energy);

(c) $F_2(L_1)$ is identical to the energy $G(L_1)$ minus $4a^2/L$;

(d) $F_3(L_1)$ can be seen as the interaction energy between f_2 and ξ.

Among these observations, (d) needs some explanations: we can see that Eq. (40) is the interaction energy between $(g - f_2) + \eta + \xi$ and f_2; then we observe that the interaction energy between $g - f_2$ and f_2 is zero because the first derivatives of the former is a constant, and the interaction energy between η and f_2 is zero because the former is nonzero only at $x = L_1$, while the latter is defined on $[0, L_1) \cup (L_1, L]$, therefore the domains are not overlapped.

The above observations explain why we can cancel $F_1(L_1)$, $F_3(L_1)$, as well as why $F_2(L_1)$ and $G(L_1)$ are equally effectively in determining the ground states. So far we are unable to provide more rigorous mathematical formulas for these observations because the derivation and integration for η and ξ are bizarre and a precise rule is unknown. However, further work needs to be done to develop these observations into criteria that are suited for a variety of similar examples, so that we do not need lengthy calculations [which leads to Eq. (43)] to figure out which part of the total energy needs to be canceled.

Now, there is a question: Method (b) seems to be much more difficult than Method (a), so why do we need it? Our answer is that: first, Method (a) can be awfully difficult for other examples; second, Method (b) seems to have a much more simplified version once we have the criteria to cancel out the unwanted part of the free energy. The simplified version of Method (b) is the following.

Step 1: Derive the expression for f with B as an unknown parameter, i.e., Eqs. (19)-(24);

Step 2: Rewrite Eq. (25) as

$$\sum_{k=1}^{\infty}\frac{4a}{k\pi}\cos\frac{k\pi L_1}{L}\sin\frac{k\pi L_1}{L} = -\sum_{k=1}^{\infty}\frac{2L}{(k\pi)^2}B\sin\frac{k\pi L_1}{L}\sin\frac{k\pi L_1}{L}. \tag{47}$$

The LHS and RHS of Eq. (47) have the same monotonicity and zero points with respect to L_1, and the first terms of the LHS and RHS are enough to determine the monotonicity and zero points. Therefore, if we are only interested in finding the ground state instead of its energy value, we just focus on the first terms of these sums. Thus, we replace Eq. (25) or (47) by

$$\frac{4a}{\pi}\cos\frac{\pi L_1}{L}\sin\frac{\pi L_1}{L} = -\frac{2L}{(\pi)^2}B\sin\frac{\pi L_1}{L}\sin\frac{\pi L_1}{L}, \tag{48}$$

therefore we have

$$B = -\frac{2\pi a}{L}\cot\frac{\pi L_1}{L}. \tag{49}$$

Notice that Eqs. (26) and (49) have the same monotonicity and zero points.

Step 3: Knowing that Eq. (39) is the sum of a convergent sequence, we observe that the first term also determines the monotonicity and zero points of the whole sum. Therefore, we substitute Eq. (49) into the first term of Eq. (39), and then we have

$$F_2(L_1) = \frac{8a^2}{L}\cos^2\frac{\pi L_1}{L}. \tag{50}$$

Interestingly, Equations (14), (39) and (50) have the same ground states, thus are equally effective for our purpose.

By comparing Eq. (50) with Eq. (38), we observe that the largest Fourier mode of the background energy determines the ground state, which could be a common feature for lots of similar examples, one of which is Example 2.

1.4 Solving Example 2 by Method (b)

By the same procedure, we have

$$f(x) = f_1(x) + f_2(x), \tag{51}$$

where

$$f_1(x) = \sum_{k=1}^{\infty}\frac{\frac{4k\pi a}{L^2}}{A^2+(\frac{k\pi}{L})^2}\cos\frac{k\pi L_1}{L}\sin\frac{k\pi x}{L}; \tag{52}$$

$$\begin{aligned} f_2(x) &= \sum_{k=1}^{\infty}\frac{2C}{L}\cdot\frac{\sin\frac{k\pi L_1}{L}}{A^2+(\frac{k\pi}{L})^2}\sin\frac{k\pi x}{L} \\ &= \sum_{k=1}^{\infty}\frac{2}{L}\cdot\frac{\sin\frac{k\pi L_1}{L}}{A^2+(\frac{k\pi}{L})^2}\Big(-Aa\cdot\frac{e^{AL_1}+e^{-AL_1}}{e^{AL_1}-e^{-AL_1}}+Aa\cdot\frac{e^{2AL-AL_1}+e^{AL_1}}{e^{2AL-AL_1}-e^{AL_1}}\Big)\sin\frac{k\pi x}{L}; \end{aligned} \tag{53}$$

and

$$F(L_1) = F_1(L_1)+F_2(L_1)+F_3(L_1)+F_4(L_1), \tag{54}$$

where

$$F_1(L_1) = \frac{1}{2L}\cdot\sum_{k=1}^{\infty}\Big(4a\cos\frac{k\pi L_1}{L}\Big)^2, \tag{55}$$

$$\begin{aligned} F_2(L_1) &= \frac{1}{2L}\cdot\sum_{k=1}^{\infty}\left[\frac{\frac{4(k\pi)^2a}{L^2}}{A^2+(\frac{k\pi}{L})^2}\cos\frac{k\pi L_1}{L}-4a\cos\frac{k\pi L_1}{L}+\frac{2C}{L}\cdot\frac{k\pi\cdot\sin\frac{k\pi L_1}{L}}{A^2+(\frac{k\pi}{L})^2}\right]^2 \\ &= \frac{1}{2L}\cdot\sum_{k=1}^{\infty}\left[\frac{\frac{4(k\pi)^2a}{L^2}}{A^2+(\frac{k\pi}{L})^2}\cos\frac{k\pi L_1}{L}-4a\cos\frac{k\pi L_1}{L}+\frac{2}{L}\right. \\ &\qquad \left.\cdot\frac{k\pi\cdot\sin\frac{k\pi L_1}{L}}{A^2+(\frac{k\pi}{L})^2}\Big(-Aa\cdot\frac{e^{AL_1}+e^{-AL_1}}{e^{AL_1}-e^{-AL_1}}+Aa\cdot\frac{e^{2AL-AL_1}+e^{AL_1}}{e^{2AL-AL_1}-e^{AL_1}}\Big)\right]^2, \end{aligned} \tag{56}$$

$$
\begin{aligned}
F_3(L_1) &= \frac{1}{L}\cdot\sum_{k=1}^{\infty}\Big(4a\cos\frac{k\pi L_1}{L}\Big)\cdot\left[\frac{\frac{4(k\pi)^2a}{L^2}}{A^2+(\frac{k\pi}{L})^2}\cos\frac{k\pi L_1}{L}-4a\cos\frac{k\pi L_1}{L}+\frac{2C}{L}\cdot\frac{k\pi\cdot\sin\frac{k\pi L_1}{L}}{A^2+(\frac{k\pi}{L})^2}\right]\\
&= \frac{1}{L}\cdot\sum_{k=1}^{\infty}\Big(4a\cos\frac{k\pi L_1}{L}\Big)\cdot\left[\frac{\frac{4(k\pi)^2a}{L^2}}{A^2+(\frac{k\pi}{L})^2}\cos\frac{k\pi L_1}{L}-4a\cos\frac{k\pi L_1}{L}+\frac{2}{L}\right.\\
&\quad\left.\cdot\frac{k\pi\cdot\sin\frac{k\pi L_1}{L}}{A^2+(\frac{k\pi}{L})^2}\Big(-Aa\cdot\frac{e^{AL_1}+e^{-AL_1}}{e^{AL_1}-e^{-AL_1}}+Aa\cdot\frac{e^{2AL-AL_1}+e^{AL_1}}{e^{2AL-AL_1}-e^{AL_1}}\Big)\right],
\end{aligned}
\tag{57}
$$

$$
\begin{aligned}
F_4(L_1) &= \int_0^L (A^2f^2)\mathrm{d}x\\
&= A^2\int_0^L \mathrm{d}x\left[\sum_{k=1}^{\infty}\frac{\frac{4k\pi a}{L^2}}{A^2+(\frac{k\pi}{L})^2}\cos\frac{k\pi L_1}{L}+\sum_{k=1}^{\infty}\frac{2C}{L}\cdot\frac{\sin\frac{k\pi L_1}{L}}{A^2+(\frac{k\pi}{L})^2}\right]^2\\
&= A^2\int_0^L \mathrm{d}x\left[\sum_{k=1}^{\infty}\frac{\frac{4k\pi a}{L^2}}{A^2+(\frac{k\pi}{L})^2}\cos\frac{k\pi L_1}{L}+\sum_{k=1}^{\infty}\frac{2}{L}\cdot\frac{\sin\frac{k\pi L_1}{L}}{A^2+(\frac{k\pi}{L})^2}\Big(\right.\\
&\quad\left.-Aa\cdot\frac{e^{AL_1}+e^{-AL_1}}{e^{AL_1}-e^{-AL_1}}+Aa\cdot\frac{e^{2AL-AL_1}+e^{AL_1}}{e^{2AL-AL_1}-e^{AL_1}}\Big)\right]^2.
\end{aligned}
\tag{58}
$$

Similarly, $F_1(L_1)$ is the background energy, $F_3(L_1)$ is the fictitious interaction energy; and $F_2(L_1)+F_4(L_1)$ is the same as Eq. (18) up to a constant, therefore is equally effective in determining the ground state.

Similar to the last section, once we know some criteria that guide us to keep only $F_2(L_1)$ and $F_4(L_1)$ with C being an unknown parameter, then the simplified calculation can be the following:

Step 1: Derive the expression for f with C as an unknown parameter, similar to Eqs. (19)-(24);

Step 2: By the fact that C is determined by $f(L_1)=0$, we have the following relation

$$
\sum_{k=1}^{\infty}\frac{\frac{4k\pi a}{L^2}}{A^2+(\frac{k\pi}{L})^2}\cos\frac{k\pi L_1}{L}\sin\frac{k\pi L_1}{L}=-\sum_{k=1}^{\infty}\frac{2C}{L}\cdot\frac{\sin\frac{k\pi L_1}{L}}{A^2+(\frac{k\pi}{L})^2}\sin\frac{k\pi L_1}{L}. \tag{59}
$$

Keep only the first term, and we have

$$
C=-\frac{2\pi a}{L}\cot\frac{\pi L_1}{L}. \tag{60}
$$

Step 3: Substitute Eq. (60) into the first term of $F_2(L_1)+F_4(L_1)$ as shown in Eqs. (56) and (58), and we have

$$
F_2(L_1)+F_4(L_1)=\frac{8a^2}{L}\cos^2\frac{\pi L_1}{L}. \tag{61}
$$

Interestingly, Equations (50) and (61) are the same, which is consistent with the fact that Example 1 and 2 have the same ground state.

1.5 Example 3

Now let us consider M discontinuities located at $(L_1,0),(L_1+L_2,0),\dots,(L_1+L_2+\cdots+L_M,0)$ with the similar energy functional as Example 1 [i.e., Eq. (1)]. Our goal is, still, to find the ground state when $L_1,L_2,\dots,L_M$ vary.

By Method (a), we have

$$f(x)=\begin{cases} -\frac{a}{L_1}x,\ x\in[0,L_1), \\ -\frac{2a}{L_2}x+\frac{2aL_1}{L_2}+a,\ x\in(L_1,L_2), \\ -\frac{2a}{L_i}x+\frac{2a}{L_i}(L_1+L_2+\cdots+{}_{i-1})+a,\ x\in(L_1+\cdots+L_{i-1},L_1+\cdots+L_{i-1}+L_i),\ i\le M, \\ \vdots \\ -\frac{a}{L-(L_1+L_2+\cdots+{}_M)}x+\frac{aL}{L-(L_1+L_2+\cdots+{}_M)},\ x\in(L_1+\cdots+{}_M,L]. \end{cases} \tag{62}$$

Therefore we have the following energy landscape

$$F(L_1,L_2,\dots,L_M)=\frac{a^2}{L_1}+\frac{4a^2}{L_2}+\cdots+\frac{4a^2}{L_i}+\cdots+\frac{4a^2}{L_M}+\frac{a^2}{L-(L_1+L_2+\cdots+L_M)}. \tag{63}$$

To find the ground state, we solve the following equations

$$\frac{\partial F}{\partial L_i}=0,\ i\in\{1,2,\dots,M\} \tag{64}$$

which is written explicitly as

$$-\frac{1}{L_1^2}+\frac{1}{[L-(L_1+L_2+\cdots+L_M)]^2}=0, \tag{65}$$

$$-\frac{4}{L_i^2}+\frac{1}{[L-(L_1+L_2+\cdots+L_M)]^2}=0,\ i\in\{2,3,\dots,M\} \tag{66}$$

Therefore, the ground state is

$$L_1=\frac{L}{2M},L_2=L_3=\cdots=L_M=\frac{L}{M}. \tag{67}$$

By Method (b), we have

$$f(x)=f_1(x)+f_2(x), \tag{68}$$

where

$$f_1(x)=\sum_{k=1}^{\infty}\Big[\frac{4a}{k\pi}\cos\frac{k\pi L_1}{L}+\frac{4a}{k\pi}\cos\frac{k\pi(L_1+L_2)}{L}+\cdots+\frac{4a}{k\pi}\cos\frac{k\pi(L_1+L_2+\cdots+L_M)}{L}\Big]\sin\frac{k\pi x}{L}, \tag{69}$$

$$\begin{aligned} f(x)=\sum_{k=1}^{\infty}\Big[&\frac{2L}{(k\pi)^2}B_1\sin\frac{k\pi L_1}{L}+\frac{2L}{(k\pi)^2}B_2\sin\frac{k\pi(L_1+L_2)}{L}+\cdots \\ &+\frac{2L}{(k\pi)^2}B_M\sin\frac{k\pi(L_1+L_2+\cdots+L_M)}{L}\Big]\sin\frac{k\pi x}{L}; \end{aligned} \tag{70}$$

and the energy function

$$F(L_1,L_2,\dots,L_M)=F_1(L_1,L_2,\dots,L_M)+F_2(L_1,L_2,\dots,L_M)+F_3(L_1,L_2,\dots,L_M), \tag{71}$$

where

$$F_1(L_1,L_2,\cdots,L_M)=\sum_{k=1}^{\infty}\frac{2}{L}\Big[2a\cos\frac{k\pi L_1}{L}+2a\cos\frac{k\pi(L_1+L_2)}{L}+\cdots+2a\cos\frac{k\pi(L_1+L_2+\cdots+L_M)}{L}\Big]^2, \tag{72}$$

$$F_2(L_1,L_2,\cdots,L_M)=\sum_{k=1}^{\infty}\frac{2}{L}\Big[\frac{L}{k\pi}B_1\sin\frac{k\pi L_1}{L}+\frac{L}{k\pi}B_2\sin\frac{k\pi(L_1+L_2)}{L}$$
$$+\cdots+\frac{L}{k\pi}B_M\sin\frac{k\pi(L_1+L_2+\cdots+L_M)}{L}\Big]^2, \tag{73}$$

$$F_3(L_1,L_2,\cdots,L_M)=\sum_{k=1}^{\infty}\frac{4}{L}\Big[2a\cos\frac{k\pi L_1}{L}+2a\cos\frac{k\pi(L_1+L_2)}{L}+\cdots$$
$$+2a\cos\frac{k\pi(L_1+L_2+\cdots+L_M)}{L}\Big]\cdot\Big[\frac{L}{k\pi}B_1\sin\frac{k\pi L_1}{L}$$
$$+\frac{L}{k\pi}B_2\sin\frac{k\pi(L_1+L_2)}{L}+\cdots+\frac{L}{k\pi}B_M\sin\frac{k\pi(L_1+L_2+\cdots+L_M)}{L}\Big]^2. \tag{74}$$

$B_1,B_2,\cdots,B_M$ are functions of $L_1,L_2,\cdots,L_M$. By the Dirichlet conditions, we have

$$f(L_1)=f(L_1+L_2)=\cdots=f(L_1+L_2+\cdots+L_M)=0, \tag{75}$$

which gives

$$B_1=\frac{2}{L_2}-\frac{1}{L_1},B_2=\frac{2}{L_3}-\frac{2}{L_2},\ldots,B_M=\frac{1}{L-(L_1+L_2+\cdots+L_M)}-\frac{2}{L_M}. \tag{76}$$

The simplified calculation does not need Eq. (76). Following the same steps as described in the last two subsections, we write Eq. (75) as Fourier series just like Eqs. (48) and (59), and we think the first N terms determine the monotonicity and zero points of the whole series. Therefore we can let $B_1,B_2,\ldots,B_M$ satisfy

$$2a\cos\frac{\pi L_1}{L}+2a\cos\frac{\pi(L_1+L_2)}{L}+2a\cos\frac{\pi(L_1+L_2+\cdots+L_M)}{L}+\cdots$$
$$+\frac{L}{\pi}B_1\sin\frac{\pi L_1}{L}+\frac{L}{\pi}B_2\sin\frac{\pi(L_1+L_2)}{L}+\cdots+\frac{L}{\pi}B_M\sin\frac{\pi(L_1+L_2+\cdots+L_M)}{L}=0, \tag{77}$$

$$2a\cos\frac{2\pi L_1}{L}+2a\cos\frac{2\pi(L_1+L_2)}{L}+2a\cos\frac{2\pi(L_1+L_2+\cdots+L_M)}{L}+\cdots+\frac{L}{2\pi}B_1\sin\frac{2\pi L_1}{L}$$
$$+\frac{L}{2\pi}B_2\sin\frac{2\pi(L_1+L_2)}{L}+\cdots+\frac{L}{2\pi}B_M\sin\frac{2\pi(L_1+L_2+\cdots+L_M)}{L}=0,$$

$\cdots\cdots$

$$2a\cos\frac{M\pi L_1}{L}+2a\cos\frac{M\pi(L_1+L_2)}{L}+2a\cos\frac{M\pi(L_1+L_2+\cdots+L_M)}{L}+\cdots+\frac{L}{M\pi}B_1\sin\frac{M\pi L_1}{L}$$
$$+\frac{L}{M\pi}B_2\sin\frac{M\pi(L_1+L_2)}{L}+\cdots+\frac{L}{M\pi}B_M\sin\frac{M\pi(L_1+L_2+\cdots+L_M)}{L}=0.$$

Then $F_2(L_1,L_2,\ldots,L_M)$ can be approximated as

$$F_2(L_1,L_2,\ldots,L_M)=\sum_{k=1}^{M}\frac{8a^2}{L}\Big[\cos\frac{k\pi L_1}{L}+\cos\frac{k\pi(L_1+L_2)}{L}+\cdots+\cos\frac{k\pi(L_1+L_2+\cdots+L_M)}{L}\Big]^2, \tag{78}$$

Thus the ground state is given by

$$\cos\frac{k\pi L_1}{L}+\cos\frac{k\pi(L_1+L_2)}{L}+\cdots+\cos\frac{k\pi(L_1+L_2+\cdots+L_M)}{L}=0,\ \forall k\in\{1,2,\ldots,M\}, \tag{79}$$

and it is exactly Eq. (67). Again, by comparing Eqs. (72) and (78), we can see that the largest few Fourier modes of the background energy determine the ground state.

2 Implications

2.1 The 2D Nematics

In the Oseen-Frank theory for the elasticity of the nematic liquid crytal, the distortion free energy functional is written as

$$F = \int \mathrm{d}^3V \Big[\frac{K_{11}}{2} (\nabla \cdot \mathbf{n})^2 + \frac{K_{22}}{2} (\mathbf{n} \cdot (\nabla \times \mathbf{n}))^2 + \frac{K_{33}}{2} (\mathbf{n} \times (\nabla \times \mathbf{n}))^2 \Big], \tag{80}$$

where $\mathbf{n}$ is a unit vector field, i.e., $|\mathbf{n}|= 1$; and $\mathbf{n}$ and $-\mathbf{n}$ are physically equivalent. For simplicity, we consider nematics confined in a rectangle of length L_1 and width L_2, and we assume $\mathbf{n}$ is perpendicular to the boundary and apply one-constant approximation, i.e., $K_{11} = K_{22} = K_{33} = K$; see Refs. [1, 2, 3].

$\mathbf{n}$ is decomposed as

$$\mathbf{n} = n_x \hat{\mathbf{x}} + n_y \hat{\mathbf{y}}. \tag{81}$$

Therefore the energy functional can be written as

$$F = K \int_0^{L_1} \mathrm{d}x \int_0^{L_2} \mathrm{d}y \, \Big[\Big(\frac{\partial n_x}{\partial x} \Big)^2 + \Big(\frac{\partial n_x}{\partial y} \Big)^2 + \Big(\frac{\partial n_y}{\partial x} \Big)^2 + \Big(\frac{\partial n_y}{\partial y} \Big)^2 \Big], \tag{82}$$

with the constraints

$$n_x^2 + n_y^2 = 1, \tag{83}$$

and $\mathbf{n}$ and $-\mathbf{n}$ are physically equivalent [4]. Thus we have the following Euler-Lagrange Equations

$$\frac{\partial^2 n_x}{\partial x^2} + \frac{\partial^2 n_x}{\partial y^2} + \Big[\Big(\frac{\partial n_x}{\partial x} \Big) + \Big(\frac{\partial n_x}{\partial y} \Big) + \Big(\frac{\partial n_y}{\partial x} \Big) + \Big(\frac{\partial n_y}{\partial y} \Big) \Big] n_x = 0, \tag{84}$$

$$\frac{\partial^2 n_y}{\partial x^2} + \frac{\partial^2 n_y}{\partial y^2} + \Big[\Big(\frac{\partial n_x}{\partial x} \Big) + \Big(\frac{\partial n_x}{\partial y} \Big) + \Big(\frac{\partial n_y}{\partial x} \Big) + \Big(\frac{\partial n_y}{\partial y} \Big) \Big] n_y = 0. \tag{85}$$

together with the boundary conditions

$$n_x(0, y) = -1, \tag{86}$$

$$n_x(L_1, y) = 1, \tag{87}$$

$$n_x(x, 0) = 0, \tag{88}$$

$$n_x(x, L_2) = 0, \tag{89}$$

$$n_y(0, y) = 0, \tag{90}$$

$$n_y(L_1, y) = 0, \tag{91}$$

$$n_y(x, 0) = -1, \tag{92}$$

$$n_y(x, L_2) = 1. \tag{93}$$

The intriguing part about Eqs. (84) and (85) is that, on one hand, they are nonlinear PDEs; on the other hand, they cannot be satisfied in the whole region due to the boundary conditions (84)-(85). The regions where Eqs. (84) and (85) are not satisfied are characterized by $|\mathbf{n}|= 0$; and for convenience, we call them singularities. In 2D nematics, they are usually points, and we call them defect cores. We define their winding numbers according to the rotation of vector fields around them, which can be integer or half integer. For our example, if there is a defect core with winding number being a half integer, there must be a line-shaped singularity connecting it to another defect core with half-integer winding number; see Refs. [1].

To study equilibrium defect structure, we may choose a special coordinate system with its coordinate singularity coinciding with the defect core, and then solve Euler-Lagrange equations written in terms of these coordinates subject to boundary conditions. It works best if the region is infinite with no boundary and the coordinate system is easy, which our example may not satisfy. However, we can use this technique to study the local structure of the defect core, and the procedure is the following:

Parametrize the vector field $\mathbf{n}$ as

$$\mathbf{n} = \cos\theta(\rho,\phi)\hat{\mathbf{x}} + \sin\theta(\rho,\phi)\hat{\mathbf{y}}, \tag{94}$$

which satisfies Eqs. (84) and (85) in the polar coordinates

$$\frac{\partial^2\theta}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial\theta}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2\theta}{\partial\phi^2} = 0. \tag{95}$$

To determine $\mathbf{n}$ in the vicinity of defect core, we expand $\theta(\rho,\phi)$ as

$$\theta(\rho,\phi) = \theta_0(\phi) + \rho\theta_1(\phi) + \rho^2\theta_2(\phi) + \ldots, \tag{96}$$

assuming ρ is small. Then substitute Eq. (96) into Eq. (95), and we have the equation for $\theta_0(\phi)$

$$\frac{\partial^2\theta_0}{\partial\phi^2} = 0. \tag{97}$$

The solution is

$$\theta_0 = m\phi + D, \tag{98}$$

where D is a constant, and m is an integer or half-integer. Equation (98) describes a local property: $\mathbf{n}$ is symmetric near the defect core, independent of its location. This local property is similar to our Examples 1-3, therefore we may use the same techniques developed in the last section.

Let us consider the winding numbers of the defect cores to be 1 or -1, then $n_x(x,y)$ and $n_y(x,y)$ can be written as

$$\begin{aligned} n_x &= \sum_{j_1=1}^{\infty} c_{j_1,0}\sin\frac{j_1\pi x}{L_1} + \sum_{j_1,k_1=1}^{\infty} c_{j_1,k_1}\sin\frac{j_1\pi x}{L_1}\cos\frac{k_1\pi y}{L_2} \\ &= \sum_{k_1=1}^{\infty} e_{0,k_1}\sin\frac{k_1\pi y}{L_2} + \sum_{j_1,k_1=1}^{\infty} e_{j_1,k_1}\cos\frac{j_1\pi x}{L_1}\sin\frac{k_1\pi y}{L_2}, \end{aligned} \tag{99}$$

$$\begin{aligned} n_y &= \sum_{j_2=1}^{\infty} d_{j_2,0}\sin\frac{j_2\pi x}{L_1} + \sum_{j_2,k_2=1}^{\infty} d_{j_2,k_2}\sin\frac{j_2\pi x}{L_1}\cos\frac{k_2\pi y}{L_2} \\ &= \sum_{k_2=1}^{\infty} f_{0,k_2}\sin\frac{k_2\pi y}{L_2} + \sum_{j_2,k_2=1}^{\infty} f_{j_2,k_2}\cos\frac{j_2\pi x}{L_1}\sin\frac{k_2\pi y}{L_2}. \end{aligned} \tag{100}$$

Then following the similar procedure as Eqs. (21)-(24), we can derive a finite set of algebraic equations that are able to represent different number and locations of defect cores. However, since there are infinite number of $c_{j,k}$, $d_{j,k}$, $e_{j,k}$ and $f_{j,k}$ which are also coupled to each other, we are not sure of how we can use our simplified calculation of Method (b) [as shown in Eqs. (47)-(50), (59)-(61) and (77)-(79)]. We guess, based on the conclusion made in the last section, that the largest few Fourier modes of the background energy (which we need to derive) determine the number and locations of the defect cores. This may be visualized as the following: imagine a single sine function with the zeros representing the defect cores; then add another sine function with much smaller amplitude and different frequency, and we can observe the change of locations of these zeros; then if we increase the amplitude of the added function, the number of zeros will eventually change.

3 Conclusions

We experimented with two methods of calculus of variations on three one-dimensional examples. The method of Fourier series has shown that the dominant Fourier modes of the background energy determine the ground states. That may imply a way of determining the ground state of nematic defects in confined geometry.

Acknowledgements

This work is motivated by the study of defects in nematic liquid-crystal capillary bridges in which the author was involved [5]. The author would like to thank Alberto Fernandez-Nieves, Perry W. Ellis and Jayalakshmi Vallamkondu for providing experimental insights. The author also thanks Paul M. Goldbart for his support, encouragement and discussions.

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