

# On the thinning of films (I)

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## Abstract

We investigate, from a mathematical perspective, the problem of a layer of fluid attracted to a horizontal plate when the layer is in equilibrium with a bulk reservoir. It is assumed that as the temperature varies, the bulk undergoes a continuous phase transition. On the basis of free energetics, this initially causes thinning of the layer but, at lower temperatures, the layer recovers and rebuilds. We provide a mathematical framework with which to investigate these problems. As an approximation, we model the layered system by a mean-field Ising magnet. The layered system is first studied in isolation (fixed thickness) and then as a system in contact with the bulk (variable thickness) with general results established. Finally, we investigate the limit of large thickness. Here, a well defined continuum theory emerges which provides an *approximation* to the discrete systems. In the context of the limiting theory, it is established that discontinuities in the layer thickness (as a function of temperature) or the derivative thereof are inevitable. By comparison with actual data from [8] and [7] the discontinuities may indeed be present but they are not quite in the form predicted by the theory. Finally – still in the context of the limiting theory – is shown that at low temperatures, the layer may be lost altogether; the nature of the critical binding force is elucidated.

# 1 Introduction: statement of the problem

The central purpose of this note is to provide, in the context of a well defined model, a statistical mechanics description of a *layered* system interacting with a substrate all of which is in the presence of a *bulk reservoir*. We will work at the level of mean-field theory. Usually “mean-field theory” indicates a spin (or particle) system where, for a finite number,  $N$ , of elements, each element interacts homogeneously and weakly with all (or many) of the other elements. Then one can investigate the thermodynamic and statistical behavior as  $N \rightarrow \infty$ . In this work, we will consider a finite ensemble of  $L$  such systems arranged in a linear fashion. Each such system should be envisioned as a  $d$ -dimensional system ( $d = 1$  or  $2$  of primary importance) with the “line” extending in an orthogonal direction. For obvious reasons we will refer to the constituent systems as *layers*. Here, the interaction may be loosely described as follows: within each layer the interaction is of the above described mean-field type and further, each spin interacts with all (or many) spins in the neighboring layers – ostensibly with a different interaction parameter. (We will briefly consider additional interactions between further neighboring layers but, for present purposes, we regard this as an unnecessary complication.) Finally there is a layer dependent chemical potential term which represents the overall affinity that the layer has for the *substrate*. This is sufficient for an informal description; the premise of this work is to figure out, on the basis of free energetics – compared to a background homogenous system (reservoir) – how many layers are present. Moreover, we stipulate without apology that each layer is fully present or absent altogether – i.e., we will not consider the systems with partial layers. The regime of interest is when the reservoir undergoes a continuous change of phase.

The models we will consider are of the Ising type. At the level of mean-field theory, we believe that this simplification is not too drastic. Indeed, it is likely that most of our results could have been derived with other mean-field models (provided that the mean-field transition is *continuous*). In particular, most other mean-field theories differ from the Ising model only via the value of various parameters. Thus, at various stages, we have substituted the particular numerical Ising parameters (e.g., couplings) with generic parameters and, in all cases, results have proved to be independent of these substitutions.

The primary motivation for this work is a series of remarkable experiments [8] [7] that has captured the thinning effects of  $^4\text{He}$  thin films suspended above a reservoir of bulk  $^4\text{He}$ . The experiments have shown that the thickness of the film remains relatively constant while the temperature is above the bulk critical temperature. However: these films (dramatically) undergo thinning as the temperature is lowered through and below  $T_c$ . Then, as the temperature continues to lower, the film will then re-thicken to a substantial fraction of its previous equilibrium length. This thinning is consistent with finite scaling theory as it exhibits data collapse [7].

Treatments of order parameter fluctuations have accurately described the thinning in the critical region just above  $T_c$  [9]. In addition, treatments of surface fluctuations in the superfluid regime have explained the residual thinning of the film [14]. What remains unresolved is the relatively large part of the thinning which takes place in the *vicinity* of the critical region. It is the opinion of the authors that the qualitative aspects this phenomena can be described by the interplay of free energies between the bulk and the film. Thus a good place to start is with a mean-field theoretic treatment using the simplest possible model. We have acquired qualitative understanding of this regime including, on the one hand a definitive prediction that some form of discontinuous behavior for the layer thickness as a function of temperature is inevitable. On the other hand, while the discontinuities are indeed present in the data, their quantitative form differs markedly from that of the predictions. In particular, here we find – necessarily – that the thinning epoch *ends* with the discontinuity whereas when discontinuities appear in the experimental data, they typically occur in the midst of the thinning process. Moreover, in the context of the current work there is no residual thinning at low temperatures, i.e., generally, the original  $T > T_c$  thickness is fully restored.

It is most likely that the discrepancies are caused by the failure of the simplistic (classical) theory to capture important (quantum) features of the superfluid low temperature state. This problem is currently under investigation by some of the authors; our current hope/speculation is that the addition of “well understood” terms – at a phenomenological or first principals level – will rectify all difficulties. However, as a form of a corollary, it would therefore seem that for an analogous set up as [8] [7] with the bulk reservoir and films undergoing a classical continuous transition – conceivably within the realm of experimental possibility – the inevitable discontinuities, etc., will also appear but here in the form predicted by the present work.

## 2 Layered systems in isolation

Here we will study a system of  $L$  interacting Ising layers. The object will be referred to as a *film* – the thickness of which is  $L$ . In this section, the thickness will be regarded as fixed and we will derive (at a certain level of mathematical standard) basic properties of this system. These will be used, in later sections to determine the nature of the film when  $L$  is allowed to adjust “dynamically” in response in changes to external parameters.

The mean-field behavior of layered spin-systems – especially Ising systems near criticality – is hardly a new subject from the physics perspective. An early reference (among those found by the authors) is [11] and, of course, there is the well known analysis in [12]. The reader is invited to the review in [6] for relevant prior information.

From a mathematical perspective, this problem has been treated recently in the context of *independent percolation* [3] and [5]; mathematical results about systems of this sort are not readily found in the literature. Many of the Ising results (old and new) have counterparts in the Bernoulli system. However notwithstanding the approach in [2] and [5] there is no *bona fide* free energy with which a percolation model can interact with an external environment. For this, a genuine interacting system is needed and we turn to the simplest example at hand.

### 2.1 The (basic) layered model

For the Ising Model, with coupling  $J$  the free energy function of the (isotropic bulk) system with magnetization  $m$  is provided by the following equation:

$$\begin{aligned}\phi_\beta(m) - \log 2 &= -\frac{\beta J}{2}m^2 + \left(\frac{1+m}{2}\right)\log\left(\frac{1+m}{2}\right) + \left(\frac{1-m}{2}\right)\log\left(\frac{1-m}{2}\right) \\ &=: -\frac{\beta J}{2}m^2 - S_I(m) - \log 2\end{aligned}\tag{2.1}$$

where, in the future, we will omit the constant from consideration so that the interesting portion of the free energy function vanishes at  $m = 0$ . This formula is easily derived by the usual considerations, and is the appropriate object for the model defined on the complete graph. C.f., [1], especially Theorem 5, for a general discussion of these points. The actual free energy of the system is obtained by minimizing  $\phi_\beta(m)$ ;

here we will deviate from standard conventions by *not* dividing out the  $\beta$ :

$$f(\beta) = \min_{m \in (-1, +1)} \phi_\beta(m). \quad (2.2)$$

The *transition* occurs at  $\beta_c = J^{-1}$  meaning that for  $\beta > \beta_c$  the above  $f$  is minimized by  $m(\beta) \neq 0$  and for  $\beta \leq \beta_c$  the optimal magnetization is zero.

Consider, now a system of interacting layers, (formally defined on  $\{1, \dots, L\}$  which we denote by  $\mathbb{L}_L$ ) and let us assume that among the layers, the only interactions are between neighboring layers. Then the appropriate free energy function is

$$\Phi_{\beta;L}(m_1, m_2, \dots, m_L) = -\frac{\beta J_0}{2} \sum_{k=1}^L m_k^2 - \beta J_1 \sum_{k=1}^{L-1} m_k m_{k+1} - \sum_k S_I(m_k). \quad (2.3)$$

where, again, we have neglected constant terms. We shall refer to this as the *basic model*. The equation for the magnetization profile – found by minimizing  $\Phi_{\beta;L}$  is readily seen to be

$$m_k = \tanh[\beta J_0 m_k + \beta J_1 (m_{k+1} + m_{k-1})] \quad (2.4)$$

where for convenience, an  $m_0 = m_{L+1} = 0$  may be envisioned. We shall abbreviate the array  $(m_1, \dots, m_L)$  by  $\underline{m}$  and often use the alternative form

$$\Phi_{\beta;L}(\underline{m}) = -\frac{b}{2} \sum_k m_k^2 - \frac{a}{2} \sum_k m_k \Delta m_k - \sum_k S_I(m_k). \quad (2.5)$$

where  $b = \beta(J_0 + 2J_1)$ ,  $a = \beta J_1$  and  $\Delta$  is notation for the discrete Laplacian:

$$\Delta m_k := (m_{k-1} + m_{k+1} - 2m_k).$$

In Eq.(2.5), all sums run from 1 to  $L$  and, again, when necessary, we assume fictitious layers at 0 and  $L + 1$  with magnetizations  $m_0 = m_{L+1} \equiv 0$ . The free energy obtained by minimizing the right side of Eq.(2.3) will be denoted by  $F_L$ . It is noted that (in addition to the  $\beta$ ) we do *not* divide out the  $L$  in the definition of  $F_L$ . Finally, for the bulk free energy associated with this problem, we will use  $\phi_\beta(m)$  as in Eq.(2.1) with the relevant  $J$  provided by

$$J = J_0 + 2J_1.$$

As our notations indicates, the main intention is to keep  $J_0$  and  $J_1$  fixed (and strictly positive) while  $\beta$  varies. We shall almost always adhere to this convention and in case of deviation, all relevant quantities will be clear from context.

While the systems defined by Eq.(2.3) will be adequate for our description of the physical processes of interest, unfortunately, we will have some uses for *general* properties shared by all systems of this sort. This will be delegated to the next subsection in the form of a massive theorem the statement(s) of which are important but the proof of which may be omitted on a preliminary reading.

## 2.2 Properties of general layered models

For the purposes of this subsection, we shall temporarily consider the generalized version of the ferromagnetic Ising layered system which is defined as follows:

Let  $\mathbb{K} = (K_{i,j} \mid i, j \in \mathbb{L}_L)$  denote an array of interactions – which include  $i = j$  with  $K_{i,j} \geq 0$ . It is assumed that the *graph* consisting of vertices  $\mathbb{L}_L$  and edges  $(i, j)$  corresponding to the non-zero  $K_{i,j}$  is a connected graph. Then, consider the free energy

$$\Phi_{\mathbb{K}}(\underline{m}) := - \sum_j S_I(m_j) - \frac{1}{2} \sum_{i,j} K_{i,j} m_i m_j \quad (2.6)$$

and the associated mean-field equation

$$m_k = \tanh\left(\sum_j K_{k,j} m_j\right) \quad (2.7)$$

The following properties hold:

**Theorem 2.1** *Consider the generalized Ising layered system as defined. Then*

- (0) *All minimizers of  $\Phi_{\mathbb{K}}$  satisfy Eq.(2.7).*
- (1) *All minimizers of  $\Phi_{\mathbb{K}}(\cdot)$  have each  $m_k$  of the same sign which hereafter, without loss of generality, will be taken to be non-negative.*
- (2) *If Eq.(2.7) has a non-trivial non-negative solution,  $\underline{m}$ , (where by non-trivial it is meant that for some  $j$ ,  $m_j > 0$ ) then for all  $k$ ,  $m_k > 0$ . In particular, this holds for the minimizer of the functional in Eq.(2.6).*
- (3) *The equation (2.7) has at most one non-trivial non-negative solution.*
- (4) *If  $\mathbb{K}' \succ \mathbb{K}$  (meaning that  $K'_{i,j} \geq K_{i,j}$  for all  $(i, j)$ ) with  $K'_{i,j}$  strictly larger than  $K_{i,j}$  for at least one pair  $(i, j)$  then if Eq.(2.7) has a non-trivial solution with the couplings  $\mathbb{K}$  it also has a non-trivial solution for the couplings  $\mathbb{K}'$  and, denoting the respective solutions by  $\underline{m}'$  and  $\underline{m}$ , for all  $k$ ,  $m'_k > m_k$ .*

(5) Regarding  $\mathbb{K}$  as a matrix (with elements  $K_{i,j}$ ) the necessary and sufficient condition for the existence of a non-trivial solution is that the maximum eigenvalue of  $\mathbb{K}$  exceed unity. Moreover, under this condition, the afore mentioned solution minimizes  $\Phi_{\mathbb{K}}(\cdot)$ .

**Remark.** For the basic model, defined by Eq.(2.3), the eigenvalue condition reads

$$\beta J_0 + 2\beta J_1 > 1 - 2\beta J_1 \lambda_0 \quad (2.8)$$

where

$$|\lambda_0| = 1 - \cos \frac{\pi}{L+1} \approx \frac{1}{2} \frac{\pi^2}{L^2} \quad (\text{for } L \gg 1). \quad (2.9)$$

Results along these lines (at least for large  $L$ ) have been known in the physics literature for quite a while; e.g., the works [11], [12] and various others; c.f., the review by [6]. However, these results are all based on linearization of the mean-field equation (Eq.(2.4) or, more precisely the Ginzburg–Landau continuum version thereof) and, e.g., do not preclude the possibility of discontinuous transitions at higher temperatures. But, in any case, these results all turn out to be essentially correct and here a complete proof is provided. It is further remarked that in the context of *layered percolation*, most of these results were established in [5] and [3] by methods which are not dissimilar. Finally, it is remarked that some of the monotonicities in the statement of Theorem 2.1 – but not necessarily their strict versions – can be derived by considering the layered model as a limit of actual Ising systems with long-range interactions. However, here we use only the basic structure of the mean-field equations thence one may anticipate that these results hold for alternative spin-systems.

*Proof.* (0). This blatantly follows by differentiation of Eq.(2.7); it is included, for completeness and to emphasize that that any property of (all) solutions to Eq.(2.7) automatically holds for (all) minimizers of Eq.(2.6).

(1). Here, we make the observation that if  $\underline{m}$  is a trial minimizer for the functional in Eq.(2.6), the free energy is only lowered by replacing each component of  $\underline{m}$  with its absolute value. Indeed, it is clear that entropy terms as well as the “diagonal” energy terms are unchanged by this transformation while the off diagonal terms are only get lowered.

(2). Suppose that  $\underline{m}$  satisfies this equation with some  $m_j \neq 0$  (and therefore positive by our convention). Examining the form of Eq.(2.7), it is clear (by positivity

of the tangent function *and* by the assumed fact that none of the other magnetizations are negative) that for all  $k$  such that  $K_{i,k} \neq 0$ ,  $m_k > 0$ . The desired result follows from the definition of a *connected graph*.

We turn to the more substantive items.

(3). By standard compactness arguments, there are always minimizers of the functional in Eq.(2.6); by (0) – (2) above, these are identically zero or componentwise positive (plus overall sign reverses which we do not discuss). We shall construct the *maximal positive solution* of Eq.(2.7) and shortly thereafter, demonstrate that, if non-trivial, it is the only positive solution of this equation. To this end, let us treat Eq.(2.7) as an iterative map:

$$\underline{m}^{[n+1]} = \underline{\Theta}(\underline{m}^{[n]}) \quad (2.10)$$

where, componentwise,

$$m_k^{[n+1]} = \Theta_k(\underline{m}) := \tanh\left(\sum_j K_{j,k} m_j\right). \quad (2.11)$$

By the afore mentioned positivity properties and other apparent monotonicity properties, the following is observed: Suppose that  $\underline{m}$  is componentwise positive and  $\underline{m}' \succ \underline{m}$  – meaning for all  $j$ ,  $m'_j \geq m_j$  – then for each  $j$ ,

$$\Theta_j(\underline{m}') \geq \Theta_j(\underline{m}) \quad (2.12)$$

i.e.,  $\underline{\Theta}(\underline{m}') \succ \underline{\Theta}(\underline{m})$ . Thus, starting at  $(1, \dots, 1)$  we obtain a non-increasing sequence that tends to a definitive limit which we denote by  $\underline{m}^*$ . Moreover, it is claimed that if  $\underline{s}$  is any other (non-negative) solution to Eq.(2.7) then  $\underline{m}^* \succ \underline{s}$ . To see this, the iterative scheme is invoked; starting with initial conditions  $\underline{s} = \underline{s}^{(0)}$  and  $(1, \dots, 1) = \underline{m}^{(0)}$ , by the above  $\underline{m}^{(n)} \succ \underline{s}^{(n)}$ ; the former converges to  $\underline{m}^*$  while the latter is identically  $\underline{s}$  and, meanwhile, the ordering holds in the limit.

Finally we show uniqueness. This is clear if  $\underline{m}^*$  is (identically) zero. Supposing otherwise, and further supposing there is an another (lower)  $\underline{s}$  which is componentwise positive satisfying Eq.(2.7). Using strict positivity of all relevant components, we can find a  $t \in (0, 1)$  for which

$$\underline{s} \succ t\underline{m}^* \quad (2.13)$$

while for at least one component – the  $j^{\text{th}}$  –

$$s_j = tm_j^*. \quad (2.14)$$

With this in mind, it is claimed that for any (fixed) non-negative  $\underline{m}$  and for any  $t$ , all the functions  $\Theta_k(t\underline{m})$  are concave in  $t$ . Moreover, each  $\Theta_k$  is strictly concave if and only if at least one the components of  $\underline{m}$  which enter are  $\Theta_k$  is non-zero. Notwithstanding the weight of the preceding statement, the result is obtained by differentiating the tangent function.

Now since  $\Theta_k(0, \dots, 0) \equiv 0$  then, by the concavity we have that for all  $k$ ,  $\Theta_k(t\underline{m}^*) > tm_k^*$ . In particular,  $\Theta_j(t\underline{m}^*)$  strictly exceeds  $r_j$  while, since it was supposed that  $t\underline{m}^* \prec \underline{s}$ , we should have  $\Theta_k(t\underline{m}^*) \leq \Theta_k(\underline{s})$  for all  $k$ .

(4). This is a direct consequence of previously employed arguments. Starting from the initial conditions  $(1, \dots, 1)$  we iterate according to Eq.(2.10) using the couplings  $\mathbb{K}$  and  $\mathbb{K}'$  to generate the sequences here denoted by  $\underline{m}^{[n]}$  and  $\underline{m}'^{[n]}$  respectively. For each  $n$ , by monotonicity of the couplings, we have  $\underline{m}^{[n]} \prec \underline{m}'^{[n]}$  and the ordering holds in the limit – which is denoted without superscript. Supposing, then that the limiting maximal  $\underline{m}$  is non-trivial then so is  $\underline{m}'$  and, indeed, for all  $j$ ,  $m'_j \geq m_j$ . Writing the fixed point equation as

$$m'_j = \Theta'_j(\underline{m}') \quad (2.15)$$

it is seen that  $m'_j \neq \Theta'_j(\underline{m})$  any time there is a  $K'_{j,k} > K_{j,k}$ . Since this was the hypothesis, there must be  $j$ 's for which  $m'_j > m_j$ . And thus, for any  $i$  “connected” to one of these  $j$ 's (by a non-zero  $(K'_{i,j})$  we have  $m'_i > m_i$ . The strict inequality for each component now follows from the assumed graph connectivity.

(5). Finally the necessary and sufficient conditions for non-trivial  $\underline{m}$ 's associated with Eq.(2.6) and Eq.(2.7): Suppose that  $\underline{m}$  is componentwise non-negative. Then, it is apparent that

$$\Theta_k(\underline{m}) \geq \sum_j K_{k,j} m_j \quad (2.16)$$

with the inequality strict whenever the right side is non-zero. Let  $\kappa$  denote the maximum eigenvalue of  $\mathbb{K}$  and suppose that  $\kappa \leq 1$ . For  $\underline{m}^*$ , the maximal solution, we multiply both sides of Eq.(2.16) by  $\underline{m}^*$  and sum. Using traditional bra-ket notation we obtain

$$\langle \underline{m}^* | \underline{m}^* \rangle \leq \langle \underline{m}^* | \mathbb{K} | \underline{m}^* \rangle \leq \kappa \langle \underline{m}^* | \underline{m}^* \rangle \quad (2.17)$$

where the first inequality is an equality if and only if  $\underline{m}^*$  is identically zero. If  $\kappa \leq 1$ , this is evidently the case.

Finally, suppose  $\kappa > 1$ . To show that  $\underline{m}^*$  is non-trivial and minimizes  $\Phi_{\mathbb{K}}(\cdot)$ , it is sufficient to show that  $\Phi_{\mathbb{K}}$  is *not* minimized by the trivial magnetization. Let  $\underline{m}^\sharp$  denote the eigenvector associated with  $\kappa$ . By the Perron–Frobenius theorem, all components of  $\underline{m}^\sharp$  are positive. Letting  $\varepsilon > 0$  (with  $\varepsilon \ll 1$ ) we have

$$\sum_k S_I(\varepsilon m_k^\sharp) = \frac{1}{2} \varepsilon^2 \langle \underline{m}^\sharp | \underline{m}^\sharp \rangle + O(\varepsilon^4) \quad (2.18)$$

while the energy term is exactly  $-\frac{1}{2} \kappa \varepsilon^2 \langle \underline{m}^\sharp | \underline{m}^\sharp \rangle$ . This is negative for  $\varepsilon$  small enough while  $\Phi_{\mathbb{K}}$  evaluated at zero magnetization profile is zero.  $\square$

### 2.3 Further properties of the basic model

We return attention to the basic model defined by Eqs. (2.3) – (2.5).

**Theorem 2.2** *If  $\underline{m}$  is a non-trivial (positive) magnetization profile which minimizes  $\Phi_{\beta;L}(\cdot)$ , the following hold:*

- (i) *The profile is symmetric about the midpoint (i.e., for  $k < L/2$ ,  $m_k = m_{L+1-k}$ ).*
- (ii) *For each  $k$ , the discrete Laplacian is pointwise negative:  $\Delta m_k < 0$*

*Proof* (i). The cases  $L$  even or odd differ only slightly; we omit full details of the even case. For  $L$  odd, let  $\ell$  denote the midpoint. We may write, for any  $\underline{m}$

$$\Phi_{\beta;L}(\underline{m}) = \Phi_{\beta;L}^{\text{Left}} + \Phi_{\beta;L}^{\text{Right}} + q_\beta(m_\ell) \quad (2.19)$$

where  $\Phi_{\beta;L}^{\text{Left}}$  accounts for all interactions involving all spins with index  $j < \ell$  as well as the interaction  $\propto m_{\ell-1} m_\ell$ , the quantity  $\Phi_{\beta;L}^{\text{Right}}$  defined similarly and  $q_\beta(m_\ell)$  accounts for all terms involving  $m_\ell$  alone. Now suppose, e.g.,  $\Phi_{\beta;L}^{\text{Left}} \leq \Phi_{\beta;L}^{\text{Right}}$ . Then we will replace the magnetizations on layers with index larger than  $\ell$  with the magnetizations of the reflection of these layers about the midpoint:

$$m_{\ell+j} \rightarrow m_{\ell-j} \quad (j < \ell). \quad (2.20)$$

Then the free energy “improves” to  $2\Phi_{\beta;L}^{\text{Left}} + q_\beta(m_\ell)$  for this symmetrized profile. In particular a minimizing profile would be symmetric which by uniqueness of the minimizer implies that *the* minimizing profile is symmetric.

The argument for the even case is almost identical: Let  $\ell = \frac{L}{2}$  and  $\ell' = \ell + 1$  denote the two ‘‘midpoints’’. We may write (using the same notation with slightly different meaning)

$$\Phi_{\beta;L}(\underline{m}) = \Phi_{\beta;L}^{\text{Left}} + \Phi_{\beta;L}^{\text{Right}} + \frac{1}{2}\beta J_1(m_\ell - m_{\ell'})^2 \quad (2.21)$$

and the argument proceeds along the same lines noting that replacing the higher half with the profile of the lower half also gets rid of the last (positive) term on the right side of Eq.(2.21)  $\square$

*Proof* (ii). Let  $k \in \mathbb{L}_L$  (our notation for the lattice of  $L$  layers) and let us focus on the portion of the free energy function that depends on  $m_k$ . We write

$$\Phi_{\beta;L}(\underline{m}) = -\frac{1}{2}\beta J_0 m_k^2 - \beta J_1(m_k m_{k-1} + m_k m_{k+1}) - S_I(m_k) + \mathcal{R}(\underline{m}) \quad (2.22)$$

where  $\mathcal{R}$  does not depend on  $m_k$  and in case  $k$  equals 1 or  $L$  we invoke  $m_0 = m_{L+1} = 0$ . Let us rewrite the  $m_k$ -dependent part denoting the result by  $p(m_k)$ :

$$\begin{aligned} p(m_k) &= -\left(\frac{1}{2}\beta J_0 + \beta J_1\right)m_k^2 - S_I(m_k) - \beta J_1(m_k m_{k-1} + m_k m_{k+1} - m_k^2) \\ &= \phi_\beta(m_k) - \beta J_1(m_k m_{k-1} + m_k m_{k+1} - m_k^2) \end{aligned} \quad (2.23)$$

Now if we change  $m_k \rightarrow m_k + \delta m_k$ , we see

$$p(m_k + \delta m_k) = \phi_\beta(m_k + \delta m_k) - \beta J_1(m_k m_{k-1} + m_k m_{k+1} - m_k^2) - 2\beta J_1(\delta m_k \Delta m_k) \quad (2.24)$$

i.e.,  $p(m_k + \delta m_k) - p(m_k) = \phi_\beta(m_k + \delta m_k) - \phi_\beta(m_k) - 2\beta J_1(\delta m_k \Delta m_k)$  while, of course,  $\mathcal{R}$  does not change. Now by item (4) in Theorem 2.1 we have that in any minimizing profile,  $m_k(\beta) < m(\beta)$  where  $m(\beta)$  is defined with coupling  $J = J_0 + 2J_1$ . (This can be seen in any number of ways – the quickest is to compare with periodic boundary conditions, i.e., to connect the first and last site which, miraculously, reproduces the magnetization of the bulk system.) Thus, if  $\Delta m_k \geq 0$ , we could (strictly) lower the free energy by increasing  $m_k$  – all the way up to  $m(\beta)$ .  $\square$

**Corollary 2.3** *If  $a$  and  $b$  (i.e.,  $\beta$ ,  $J_0$  and  $J_1$ ) are such that  $\Phi_\beta(\cdot)$  is minimized by a non-trivial (positive)  $\underline{m}$  then the maximum magnetization occurs at the center(s). In particular, the magnetizations  $m_k(\beta)$  rise from their lowest value at  $k = 1$  in a strictly monotone fashion till the ‘‘center’’ whereupon they fall, symmetrically, as one moves from the center to  $k = L$ .*

*Proof.* Since  $m_k$  is symmetric as a function of  $k$ , it is clear that the center must be some form of local extremum. Since  $\Delta m_k < 0$  for all  $k$  and (as is not hard to see) the discrete analog of the usual elementary result holds, it follows that the center must be a local maximum. Again invoking  $\Delta m_k < 0$ , there can be no local minima anywhere aside from the endpoints so it follows that the center is *the* maximum. The remainder of the statements follow directly from the above (i) and (ii).  $\square$

Our final result of this subsection will be of pertinence for the large  $L$  systems.

**Proposition 2.4** *Let  $b = 1 + a|\lambda_0| + gL^{-2}$  with  $g > 0$  and with  $b$  and  $a$  as defined in Eq.(2.5),  $\lambda_0$  in Eq.(2.9) and, explicitly,  $J_0$  and  $J_1$  strictly positive. Moreover, the quantity  $gL^{-2}$  is considered, one way or the other to be “small”. Then the magnetization is positive. In particular, uniformly in  $L$ , for  $L$  sufficiently large,*

$$m_\ell > [\text{const.}]gL^{-1}$$

*Proof.* For  $L$ 's that are of order unity (i.e., any *particular*  $L$ ) positivity of the magnetization is the content of item (5) in Theorem 2.1. Of pertinence here is a statement that is uniform in  $L$ .

Our opening claim is that for  $\mu < m(\beta)$ , with  $\beta$  sufficiently close to (bulk) criticality, the following holds: The free energy of the system on  $\mathbb{L}_L$  which has been constrained so that each  $m_k$  does not exceed  $\mu$ , is less than  $L\phi_\beta(\mu)$ .

Foremost, for each  $\underline{m}$  on  $\mathbb{L}_L$ , it is clear that the free energy is only lowered if we couple the first and last sites (with strength  $J_1$ ) which, as mentioned earlier, restores the finite system to the effective status of the bulk. Now for fixed  $m_{k\pm 1} \leq \mu$ , the free energy associated with the  $k^{\text{th}}$  site (c.f. Eq.(2.23)) is, as a function of  $m_k$ ,

$$-S(m_k) - \left[ \frac{1}{2}\beta J_0 m_k^2 + \beta J_1 m_k m_{k+1} + \beta J_1 m_k m_{k-1} \right]$$

where here, if  $k$  is an endpoint, we adhere to the notation of *periodic* boundary conditions. From the above equation, it is obvious, that, as far as  $m_k$  is concerned the free energy is minimized when  $m_{k\pm 1}$  take on the maximum possible value. Thus, the associated mean-field equation for  $m_k$  is

$$R(m_k) = \kappa b m_k + (1 - \kappa) b \mu \tag{2.25}$$

where  $R(x) = \text{Arctanh}x = x + \frac{1}{3}x^3 + \dots$  and  $\kappa = J_0/(J_0 + 2J_1)$ . We now show that for  $\mu < m(\beta)$ , the solution of Eq.(2.25) actually *exceeds*  $\mu$ . Thus the constrained free

energy is (still) decreasing at  $m_k = \mu$  implying (with the addition of the couplings between 1 &  $L$ ) that *all* magnetizations should saturate the constraint.

To make good on the above, let  $\theta = \theta(\mu)$  denote the solution to Eq.(2.25)

$$R(\theta) = \kappa b\mu + (1 - \kappa)b\theta. \quad (2.26)$$

Since it is assumed that  $\mu < m(\beta)$  we have that

$$R(\mu) < \mu = \kappa b\mu + (1 - \kappa)b\mu. \quad (2.27)$$

Subtracting, we have  $R(\mu) - (1 - \kappa)\mu \leq R(\theta) - (1 - \kappa)\theta$ .

Here and only here we make the “large  $L$ ” assumption. In particular, it is stipulated that  $L$  is so large that  $(1 - \kappa)b < 1$ . In that case the function  $R(x) - (1 - \kappa)x$  is monotone and the preceding inequality obtained from Eqs.(2.26) and (2.27) imply  $\theta(\mu) > \mu$ .

Thus, under the above constraint, the free energy of the system is greater than  $L\phi_\beta(\mu)$  which in turn is always in excess of the expansion to quadratic order (in  $\mu$ ):

$$L\phi_\beta(\mu) > -\frac{1}{2}[a|\lambda_0| + gL^{-2}]\mu^2 \quad (2.28)$$

This will be contrasted with an estimate of the free energy which is achieved by a calculation up to quartic order (notwithstanding that the details of certain numerical coefficients are unimportant). Here we use the lowest eigenfunction of the Laplacian:

$$m_k = \varepsilon \sin\left[\frac{k\pi}{L+1}\right]$$

with  $\varepsilon$  unknown (but small). Collecting all quadratic terms we find

$$\begin{aligned} \Phi_{\beta;L}(\underline{m}) &= \varepsilon^2 \times \left[ \frac{1}{2} \sum_k m_k^2 - \frac{b}{2} \sum_k m_k^2 - \frac{a}{2} \sum_k m_k \Delta m_k + O(\varepsilon^2) \right] \\ &= -\frac{\varepsilon^2}{2} \left[ 1 + |\lambda_0|a + \frac{g}{L^2} - 1 - |\lambda_0|a \right] \sum_k m_k^2 + O(\varepsilon^4) \\ &= -\frac{1}{4}\varepsilon^2(L+1)\frac{g}{L^2} + O(\varepsilon^4). \end{aligned} \quad (2.29)$$

Meanwhile, the quartic order is simply

$$\frac{1}{12}\varepsilon^4 \sum_k m_k^4 = \frac{1}{2}\varepsilon^4(L+1)$$

So, to leading order in  $g/L^2$  the free energy is (less than)  $-\frac{1}{4}(L+1)g^2/L^4$ . Thus, it is seen that the actual magnetization at the midpoint exceeds  $\tilde{\mu}^*$  which satisfies

$$\frac{1}{2} \frac{g^2}{L^2} [1 + O(gL^{-2})] \frac{1}{a|\lambda_0| + g/L^2} = [\tilde{\mu}^* L]^2 \quad (2.30)$$

which amounts to the claimed statement.  $\square$

### 3 Discrete layered systems above a bulk

#### 3.1 Quantities of interest, conventions

We let  $V(x)$  denote the potential energy of attraction to the plate as a function the distance from the plate. In range of interest,  $V \leq 0$  and is monotone increasing.

The binding energy for the  $L^{\text{th}}$  layer will be denoted by  $c_L$  and is defined by

$$c_L = V(a_0 L) + \mu_a g H \quad (3.1)$$

where  $a_0$  is the spacing between (centers of) layers and  $\mu_a$  is the atomic mass.

It is observed that since  $V$  goes to zero, the  $c_L$  will eventually change sign. It seems clear that the maximum possible layer thickness is precisely where this happens and so we define:

**Definition 3.1** *The quantity  $L_0$  is defined as*

$$L_0 = \max\{L \mid c_L \leq 0\} \quad (3.2)$$

A formal proof of the sentence preceding this definition will emerge when we have stated the criterion for the *equilibrium layer thickness*.

The physical setup that we are modeling envisions that the material in each layer must be removed from the bulk at a free energy cost of  $f(\beta)$  (per area) for each layer. For  $L$  layers, this is offset by  $F_L(\beta)$  (the layer free energy at the stated couplings) plus the total energetic gain for binding – including the gravitational cost – here denoted by  $C_L$ :

$$C_L = \sum_{J=0}^L c_J. \quad (3.3)$$

Thus, the gain – or cost depending on sign – for  $L$  layers will be

$$\mathbb{D}_L = F_L(\beta) + \beta C_L - Lf(\beta) \quad (3.4)$$

The equilibrium layer thickness is determined by the minimizer of  $\mathbb{D}_L$ :

$$L_\beta = \text{ARGMIN}(\mathbb{D}_L). \quad (3.5)$$

It is noted that for  $\beta = 0$  (where the above holds in a limiting sense) we have  $F_L(\beta) \equiv Lf(\beta)$  ( $= 0$ ) and thus the nomenclature  $L_0$  is actually appropriate. In the context of mean-field theory, we have  $F_L \equiv Lf(\beta)$  ( $= 0$ ) down to the bulk critical temperature which, in consequence, determines the starting point of the analysis.

### 3.2 Preliminary results

In this subsection, we establish basic properties of the discrete system. Our first results concern elementary properties of  $L_\beta$ :

**Proposition 3.2** *Consider the minimization problem as defined in and prior to Eq.(3.5) and let  $L_0$  be as defined in Eq.(3.2) (which we tacitly assume has a non-frivolous value, e.g.,  $L_0 \geq 3$ ). Then (1) For all  $\beta$ ,  $L_\beta \leq L_0$ . (2) For  $\beta \leq \beta_c$ ,  $L_\beta \equiv L_0$ . Finally: (3a) If  $|C_{L_0}| \geq J_1$  then*

$$\lim_{\beta \rightarrow \infty} L_\beta = L_0$$

*if  $c_{L_0} > 0$  and, in case  $c_{L_0}$  is exactly zero, the limit is  $L_0 - 1$ .*

*(3b) If  $|C_{L_0}| < J_1$  then*

$$\lim_{\beta \rightarrow \infty} L_\beta = 0$$

Before our proof of Propositions 3.2 we will establish an auxiliary property of the layered systems which we will state as a separate lemma.

**Lemma 3.3** *For  $L \geq 2$  and let  $m_\ell(L)$  denote the maximum (midpoint) magnetization for the system on  $\mathbb{L}_L$ . Then*

$$\phi_\beta(m_\ell(L)) \geq F_{L+1}(\beta) - F_L(\beta) \geq \phi_\beta(m_\ell(L+1))$$

*In particular then,  $F_{L+1}(\beta) - F_L(\beta) \geq f(\beta)$ .*

*Proof.* We start with the upper bound. Consider the system on  $\mathbb{L}_{L+1}$  and let  $\ell$  denote the index of the midpoint(s) with the magnetization  $m_\ell = m_\ell(L+1)$ . We shall remove this magnetization/layer and, after recombination, use the array of magnetizations with  $m_\ell$  removed as a trial function for  $F_L$ .

The entropy associated with this layer is just  $S(m_\ell)$ . All terms involving  $m_\ell$  in the energetics are

$$\Delta_{\mathcal{E}}^- = \frac{1}{2}\beta J_0 m_\ell^2 + \beta J_1 m_\ell m_{\ell-1} + \beta J_1 m_\ell m_{\ell+1} \quad (3.6)$$

all of which will be “lost”. There will be an energy “gain” from the coupling of the layers  $\ell \pm 1$  which is given by

$$\Delta_{\mathcal{E}}^+ = \beta J_1 m_{\ell-1} m_{\ell+1}. \quad (3.7)$$

Consider, then  $\Phi_{\beta;L}(\underline{m}')$  where  $\underline{m}'$  is the equilibrium magnetization profile for  $\mathbb{L}_{L+1}$  with  $m_\ell$  deleted. Then

$$F_{L+1} = \Phi_{\beta;L}(\underline{m}') + \Delta_{\mathcal{E}}^+ - \Delta_{\mathcal{E}}^- - S(m_\ell). \quad (3.8)$$

Let us note that

$$\begin{aligned} \Delta_{\mathcal{E}}^- - \Delta_{\mathcal{E}}^+ - \frac{1}{2}\beta J_0 m_\ell^2 - \beta J_1 m_\ell^2 &= -\beta J_1 (m_{\ell-1} m_{\ell+1} + m_\ell^2 - m_\ell m_{\ell+1} - m_\ell m_{\ell-1}) \\ &= -\beta J_1 (m_\ell - m_{\ell-1})(m_\ell - m_{\ell+1}) \leq 0 \end{aligned} \quad (3.9)$$

Since (by Theorem 2.2 and Corollary 2.3)  $m_\ell$  may be presumed to be the maximum magnetization on  $\mathbb{L}_{L+1}$ . Thus Eq.(3.8) can be replaced with the inequality

$$F_{L+1} \geq \Phi_{\beta;L}(\underline{m}') - S(m_\ell) - \left(\frac{1}{2}\beta J_0 + \beta J_1\right)m_\ell^2 \quad (3.10)$$

The last two terms on the right add up to precisely  $\phi_\beta(m_\ell)$  while  $\Phi_{\beta;L}(\underline{m}')$  is certainly not smaller than  $F_L$ . The lower bound has been proved.

The proof is similar for the other bound. Here working the direction  $L \rightarrow L+1$  we will insert the maximum magnetization,  $m_\ell(L)$  into the midpoint of the array on  $\mathbb{L}_L$  (i.e., a repeat) thereby obtaining a trial function for  $F_{L+1}$ . We will abbreviate  $m_\ell = m_\ell(L)$  hoping this will not cause confusion with the notation from the first half of this proof.

The calculations are similar – albeit easier – so shall be succinct. We have that  $m_\ell \geq m_{\ell+1}$ . We insert the new magnetization/layer *between* the layers  $\ell$  and  $\ell + 1$ . The result, using  $\tilde{m}$  as notation for the so described array of  $L + 1$  magnetizations is

$$\begin{aligned}\Phi_{\beta;L+1}(\tilde{m}) &= F_L + \beta J_1 m_\ell m_{\ell+1} - \beta J_1 m_\ell m_{\ell+1} - \frac{1}{2} \beta J_1 m_\ell m_\ell - \frac{1}{2} \beta J_0 m_\ell^2 - S_I(m_\ell) \\ &= F_L + \phi_\beta(m_\ell).\end{aligned}\tag{3.11}$$

Thus, the right side is an upper bound on  $F_{L+1}$  and so and the other bound is proved.  $\square$

We pause for an additional result along these lines (which is not strictly necessary for the up and coming and can be omitted on a preliminary reading). What follows is a discrete concavity result concerning the free energy of layered systems:

**Lemma 3.4** *For the layered systems with  $L \geq 2$ ,*

$$F_{L+2} - F_{L+1} \leq F_{L+1} - F_L.$$

*Proof.* We will establish that  $F_{L+2} + F_L \leq 2F_{L+1}$  by transference of a layer from one copy of  $\mathbb{L}_{L+1}$  to another thereby obtaining an upper bound on  $F_{L+2} + F_L$ . Let  $\ell$  denote the position of the maximum magnetization on  $\mathbb{L}_{L+1}$ . Then, transferring this layer to the other copy of  $\mathbb{L}_{L+1}$  between the  $\ell - 1^{\text{st}}$  and  $\ell^{\text{th}}$  layer, we obtain that the quantity

$$2F_{L+1} - \beta J_1 [-(m_\ell m_{\ell+1} + m_\ell m_{\ell+1} - m_{\ell+1} m_{\ell+1}) + (m_\ell^2 + m_\ell m_{\ell+1} - m_\ell m_{\ell+1})]$$

is an upper bound on  $F_{L+2} + F_L$ . However the correction to  $2F_{L+1}$  is seen to be  $-\beta J_1 (m_\ell - m_{\ell+1})(m_\ell - m_{\ell-1})$  which is not positive and the result is established.  $\square$

**Remark 1** The preceding is “not good news” from the analytic perspective since it means that a sign change of the discrete derivative of  $\mathbb{D}_L$  is not a sufficient condition for  $L = L_\beta$ : this concavity of the  $F_L$ ’s implies that there may be several sign changes. In particular, in the context of the large  $L_0$ -theory, several local minima may be present with the global minimizer shifting (discontinuously) as the temperature varies. Evidently these behaviors will also manifest in the discrete systems.

*Proof of Proposition 3.2.* Let  $L > L_0$  then

$$F_L + \beta C_L = F_{L_0} + (F_L - F_{L_0}) + \beta C_{L_0} + \beta \sum_{J=L_0+1}^L c_J \quad (3.12)$$

Now by (several iterations of) Lemma 3.3,  $F_L - F_{L_0} \geq (L - L_0)f(\beta)$  and, by definition of  $L_0$ , each  $c_J$  participating in the above sum is positive. Thus

$$F_L + \beta C_L - Lf(\beta) > F_{L_0} + \beta C_{L_0} - L_0f(\beta) \quad (3.13)$$

and hence  $L \neq L_\beta$  which proves the first statement.

As for the second: for  $\beta \leq \beta_c$ ,  $F_L - Lf(\beta) \equiv 0$  so  $\mathbb{D}_L = \beta C_L$  and the minimum is clearly at  $L = L_0$ .

Finally, for any  $L \geq 3$ ,  $\mathbb{D}_L - \mathbb{D}_{L-1}$  provides

$$\mathbb{D}_L - \mathbb{D}_{L-1} = F_L - F_{L-1} + \beta c_L - f(\beta) \leq \phi_\beta(m_\ell) - f(\beta) + \beta c_L \quad (3.14)$$

Note that as  $\beta \rightarrow \infty$  both  $m(\beta)$  and  $m_\ell(\beta)$  tend to one and it follows easily that  $\beta^{-1}|\phi_\beta(m_\ell) - f(\beta)| \rightarrow 0$ . Thus if  $c_L < 0$  then for all  $\beta$  sufficiently large,  $\mathbb{D}_L < \mathbb{D}_{L-1}$  which implies (assuming, of course  $L_\beta \leq L_0$ ) that among all possible candidates for minimizers with  $L \geq 3$  the best option is  $L_0$  if  $c_{L_0} < 0$  and  $L_0 - 1$  (since the magnetization is never quite equal to unity) if  $c_{L_0}$  happens to be exactly zero.

A similar, explicit calculation shows (assuming  $c_2 < 0$ ) that for  $\beta \gg 1$ ,  $\mathbb{D}_2 < \mathbb{D}_1$ . Thus if for  $\beta$  large and we find  $\mathbb{D}_1 < \mathbb{D}_0 \equiv 0$ , we are done while if  $\mathbb{D}_1 > 0$ , we are down to a comparison of zero (AKA  $\mathbb{D}_0$ ) and  $\mathbb{D}_{L_0}$ .

For large  $\beta$  asymptotics, the difference between bulk and layered free energies is almost completely accounted for by the energetics associated with the “missing coupling” in the layered system. In particular for  $L \geq 1$

$$F_L - Lf(\beta) < J_1 \beta m^2 \quad (3.15)$$

obtained e.g., by using  $m_k \equiv m(\beta)$  as a trial and a similar lower bound obtained by the reverse substitution. Hence

$$\lim_{\beta \rightarrow \infty} \frac{1}{\beta} [F_L - Lf(\beta)] = J_1.$$

Thus if  $J_1 > |C_{L_0}|$ , then  $\lim_{\beta \rightarrow \infty} L_\beta = 0$  while if  $J_1 \leq |C_{L_0}|$  we acquire the above discussed options – usually  $L_0$ . Note that the case of equality (again, highly “unlikely”) we do not get  $L_\beta \rightarrow 0$  in light of the strict inequality in Eq.(3.15) and the fact that for finite  $\beta$  the magnetization is never quite unity.  $\square$

**Remark 2** We remark that comparisons between substrate – Helium interaction energies (of the order of many degrees) versus the relevant “coupling” energies for superfluids (of the order of a few degrees) obviously demonstrate that the  $L_\beta \rightarrow 0$  scenario is not within the realm of interest for the setups in [8] and [7]. However, a remnant of this mathematical phenomenon will reemerge when we discuss the large  $L_0$  theory where numerical differences between parameters can be washed out by scaling and/or, arguably, large  $\beta$  is never reached.

Aside from the generalities described in this section, it is apparent that whenever  $L_0$  itself is of order unity the layered problems must be treated on a case by case basis with the outcome depending in a complicated way on the specifics of the model. (It also calls into question the use of mean-field theory with Ising interactions.) Moreover it would seem that actual systems with moderate  $L_0$  would be difficult to investigate experimentally. However (and fortunately) the experiments in [8] and [7] indicate the need for a large  $L_0$ -theory which will be the subject of the next subsection.

## 4 Large $L_0$ theory

As discussed above, many disparate behaviors are possible when the initial number of layers,  $L_0$ , is of order unity. Here (and in the next section) we wish to describe emergent behavior for systems with  $L_0 \gg 1$ . In the current section we will discuss, on a mathematically informal level how we arrive at the theory governing the  $L_0 = \infty$  limit and explore analytically (AKA rigorously) the asymptotic possibilities. In the next section, we will provide the mathematical underpinnings which tie the finite but large  $L_0$  models to this  $L_0 = \infty$  limit.

### 4.1 Large $L_0$ preliminaries

As will emerge in this subsection, the basis for a large  $L_0$  theory is that (at least in the range of interest)  $C_L \sim L^{-3}$ . Thus, we may as well assume  $c_L$  has the scaling of  $L_0^{-4}$  times a regular function of  $L/L_0$ . This latter variable will be  $r$ . Thus, for  $r \in (0, 1]$  we define  $c(r)$  via

$$c(r) = \lim_{L_0 \rightarrow \infty} L_0^4 c_{[rL_0]} \quad (4.1)$$

i.e.,

$$c_L \sim \frac{1}{L_0^4} c\left(\frac{L}{L_0}\right). \quad (4.2)$$

It is remarked that, from an alternative perspective, the large  $L_0$  theory can also be viewed in terms of a small  $a_0$  theory which provides a modicum of justification for an ansatz along the above lines.

We are still assuming  $c$  is increasing, let us for once and all make the stronger assumptions that  $c(r)$  is *strictly* increasing on  $(0, 1]$  with  $c(1) = 0$ . (Thus,  $c(r) < 0$  for  $r < 1$ ). Also, there is no real loss in generality to assume that  $c$  is smooth on  $(0, 1]$  but, as we shall see, it is pertinent to allow versions of  $c$  which diverge as  $r \rightarrow 0$ .

Notwithstanding the supposed existence of a non-trivial limiting  $c(r)$ , the limit thinning problem may end up, in essence, to be a triviality or (worse) exhibit behavior that is highly unlikely from a physical perspective. These possibility will be offset by a condition we refer to as the *strong wetting condition*. In its initial rendition, it has the appearance of a mathematically sufficient criterion for non-triviality which, moreover, has as much to do with the parameters  $J_0$  and  $J_1$  of the Hamiltonian as with  $c(r)$  itself. E.g., with fixed  $J_0$  and  $J_1$ , if  $c_0(r)$  satisfies the monotonicity criteria then the system is strong wetting for  $c(r) = Hc_0(r)$  for all  $H$  sufficiently large. However, as the story plays out, something even stringer is required (at  $r \ll 1$ ) in order to prevent the layer from washing out altogether at low temperature parameter. (This leads to the sharp result stated in the abstract.) Notwithstanding, the precise statement of the strong wetting condition is somewhat arduous and will be postponed till it is sufficiently motivated. If anxious, the reader is invited to Definition 4.3.

It turns out that under the strong(er) wetting condition, in the context of the large but finite  $L_0$  problems, the *entire* thinning and recovery procedure takes place in the temperature range provided by  $\beta - \beta_c$  of the order  $L_0^{-2}$ . Thus we write

$$\beta - \beta_c = \frac{B}{L_0^2} \frac{1}{J_0 + 2J_1} \quad (4.3)$$

with the scaling factor of the  $J$ 's for continued convenience. In the  $a / b$  language, this reads  $b = 1 + \frac{B}{L_0^2}$  – the scaling unveiled in Proposition 2.4.

The goal of this section will be to construct and analyze the asymptotic layered model for  $L_0 \rightarrow \infty$ , as  $B$  ranges in  $[0, \infty)$ . In the large  $L_0$  limit, with the temperature scaling as in Eq.(4.3) above, the correct scaling for the magnetization is  $m(\beta) \sim$

$(\beta - \beta_c)^{1/2} \sim L_0^{-1}$ ; we define  $M(B) = \lim_{L_0 \rightarrow \infty} L_0 m(\beta(B))$ . Then the well known result is  $M = \sqrt{3B}$ . Moreover, the the free energy change (in the bulk) scales like the fourth power of the magnetization, i.e.,  $L_0^{-4}$  which, it is noted, is compatible with the definition of  $c(r)$  provided by Eq.(4.1). In particular, for  $M \in \mathbb{R}$  of order unity and  $\beta(B)$  as described in Eq.(4.3), we make the following definitions:

$$\varphi_B(M) := \lim_{L_0 \rightarrow \infty} L_0^4 \phi(L_0^{-1} M) \quad (4.4)$$

and

$$f_B := \varphi_B(M(B)). \quad (4.5)$$

The results are  $\varphi_B(M) = -\frac{1}{2}BM^2 + \frac{1}{12}M^4$  and  $f_B = -\frac{3}{4}B^2$ .

These formulae are beset with numerical coefficients which depend on the *Ising* nature of the mean-field interaction and do not play a major rôle. Indeed, the principal difference between the Ising and other spin-systems, at this level of approximation, is the coefficient in front of the quartic term. Thus, for computational ease and to demonstrate that the conclusions reached do not depend on the Ising nature of the interaction (and to provide the reader with a familiar look) we shall replace a 3 in the quartic coefficient with  $U^{-1}$ . We thus get

$$\varphi_B(M) = -\frac{1}{2}BM^2 + \frac{1}{4}UM^4 \quad (4.6)$$

so that

$$M(B) = \sqrt{\frac{B}{U}} \quad (4.7)$$

resulting in

$$f_B = -\frac{1}{4} \frac{B^2}{U}. \quad (4.8)$$

Finally, let us tend to the object of principal interest,  $L_\beta$  that was defined in Eq.(3.5). Ultimately one is interested in the rescaled version of  $L_\beta$  namely

$$\tilde{r}_B = \lim_{L_0 \rightarrow \infty} \frac{L_\beta}{L_0}. \quad (4.9)$$

The existence of this limit, which is not *a priori* obvious will be a subject of the mathematical section and will be proved as the final result of this note (Corollary to Proposition 5.2). In this section we will be content with the object, denoted by an unadorned  $r_B$ , which is associated with the *continuum thinning model* and which, ultimately, provides the value of the limit.

## 4.2 The continuum thinning model

We now turn attention to the detailed situation in the large  $L_0$  limit. We shall begin in the discrete system and derive a certain limiting system; as is not *too* surprising the result is the standard Ginzburg–Landau model appropriate for a 1D inhomogeneous medium. We remind (and will continue to remind) the reader that the current section is informal; rigorous details will be provided in the next section.

Starting from the mean–field equation (Eq.(2.4) in the language of Eq.(2.5)) we have

$$bm_k + a\Delta m_k = \text{Arctanh}(m_k) = m_k + \frac{1}{3}m_k^3 + \dots \quad (4.10)$$

Using the appropriate scaling with  $L_0$  described previously, for  $x \in [0, 1]$ , we define  $M_B(x)$  by

$$m_k = L_0^{-1}M_B(kL_0^{-1})$$

using smooth interpolation if protocol requires. We write  $b = 1 + L_0^{-2}B$  and  $a \approx \frac{J_1}{J_0+2J_1} =: A$  and obtain

$$m_k + \frac{1}{L_0^3}BM_B + A\frac{1}{L_0^3}M_B'' = m_k + \frac{1}{3}\frac{1}{L_0^3}M_B^3 + \dots \quad (4.11)$$

so (with full justification coming later) as  $L_0 \rightarrow \infty$  we have

$$AM_B'' + BM_B - UM_B^3 = 0. \quad (4.12)$$

where, we remind the reader, we have replaced the Ising value of  $\frac{1}{3}$  with a traditional  $U$ .

It is noted that Eq.(4.12) is the Euler–Lagrange equation for the functional

$$\mathcal{F}_B(r) = \inf_{M_B} \int_0^r \left( \frac{1}{2}AM_B'^2 - \frac{1}{2}BM_B^2 + \frac{1}{4}UM_B^4 \right) dx. \quad (4.13)$$

While, from a certain perspective, it is clear that the functional on the right side of Eq.(4.13) is the correct object for the continuum theory, a proof requires some small effort. Indeed, we will show, in the Corollary to Theorem 5.1 and Proposition 5.2 that

$$\mathcal{F}_B(r) = \lim_{L_0 \rightarrow \infty} L_0^3 F_{[rL_0]}^3 \quad (4.14)$$

which is more than enough for present purposes.

We further define  $C(r)$  either directly out of  $C_L$  and/or as the integral of  $c$ :

$$C(r) = \int_{\varepsilon_0}^r c(r') dr' \quad (4.15)$$

where the lower limit indicates that some care must be taken if the divergence of  $c$  at the origin is too strong. This subject matter will be discussed in more detail in Subsection 4.4 and, in any case, will not usually be of direct concern till we discuss  $B \gg 1$ . For the present, we will suppress the presence of cutoffs in our notation.

Thus, we obtain the continuum version of the layering problem:

$$\mathcal{D}_B(r) = C(r) + \mathcal{F}_B(r) - r f_B$$

and then

$$r_B = \text{ARGMIN}(\mathcal{D}_B(r)). \quad (4.16)$$

In light of the upper and lower bounds that were proved in the discrete context in Proposition 3.3, it “must” be the case that

$$\frac{\partial \mathcal{F}_B}{\partial r} = \varphi_B(M_\ell(r, B)).$$

where  $M_\ell(r, B)$  denotes the value of the minimizer for the functional in Eq.(4.13) evaluated at the midpoint. This turns out to be the case and later (Corollary 4.2) will be derived on the basis of the functional alone. With the above in mind, a derivative condition which is a necessary but *not* sufficient condition for the determination of  $r_B$  reads:

$$c(r_B) + \varphi_B(M_\ell(r, B)) = f_B.$$

The principal result of this section is contained in the up and coming theorem. It is remarked that the forthcoming is completely rigorous under the assumption that various functions are “smooth enough” to employ classical analysis. A primary objective of Section 5 is to demonstrate that the classical solution obtained here is indeed the only mathematical possibility and indeed minimizes the functional in Eq.(4.13).

**Theorem 4.1** *Let  $M_\ell(r, B)$  denote the magnetization at the midpoint of the rescaled system on  $[0, r]$ . Then under the assumption that the functional defined in Eq.(4.13) has a classical minimizer, the following holds:*

There is a function  $\mu_\ell(Q)$  taking values in  $[0, 1)$  with argument  $Q$  in  $[0, \infty)$  – and the  $\ell$  for decoration – such that

$$M_\ell(r, B) = [\mu_\ell(A^{-1}r^2B)]M(B)$$

Moreover,  $\mu_\ell(Q)$  has the properties

- $\mu_\ell(Q)$  is monotone nondecreasing.
- $\mu_\ell \equiv 0$  for  $Q \leq \pi^2$ ;  $\mu_\ell > 0$  for  $Q > \pi^2$ .
- $\mu_\ell \rightarrow 1$  as  $Q \rightarrow \infty$ . In particular,  $\mu_\ell(Q) \sim 1 - e^{-\sqrt{Q/2}}$  for large  $Q$ .

**Remark 3** Our analysis of Eq.(4.12) will provide the proof of the above stated theorem. Much of what is to follow, not to mention the up and coming Lemma 4.7 could (we presume) be gleaned from the vast ancient literature on the subject of *elliptic* functions. However, this might only supply marginal insight into the problem at hand and, in any case, our proofs are elementary.

*Proof.* The proof comes from the investigation of the functional defined on the right hand side of Eq.(4.13). The first step is to write this functional in dimensionless form: For  $y \in [0, 1]$  let  $\mu(y)$  be defined by

$$M_B(x) = M\mu\left(\frac{x}{r}\right). \tag{4.17}$$

Then the integrand in Eq.(4.13) reads

$$A \frac{B}{U} \frac{1}{r^2} \left( \frac{1}{2}(\mu')^2 - \frac{1}{2} \frac{Br^2}{A} \mu^2 + \frac{1}{4} \frac{Br^2}{A} \mu^4 \right)$$

where the argument of  $\mu$  is still  $x/r$  and the integration is on  $[0, r]$  (so we will gain a further factor of  $r$  from the change of variables). We arrive at

$$\begin{aligned} \mathcal{F}_B(r) &= \frac{AB}{rU} \inf_{\mu} \int_0^1 \frac{1}{2}(\mu')^2 - \frac{1}{2}Q\mu^2 + \frac{1}{4}Q\mu^4 dx \\ &=: \frac{AB}{rU} \inf_{\mu} \int_0^1 \mathcal{L}_Q(\mu) dx \end{aligned} \tag{4.18}$$

where

$$Q := \frac{Br^2}{A}.$$

The object of interest in Theorem 4.1 is just

$$\mu_\ell(Q) := \mu(Q; \frac{1}{2}).$$

The proof of the first claim is the continuum version of the proof for the corresponding result in the discrete model. We shall be brief. The continuum analog of the eigenvalue condition – sometimes known as the Poincaré inequality – here reads

$$\int_0^1 (\mu')^2 dx \geq \pi^2 \int_0^1 \mu^2 dx$$

(which, in this context, is derived pretty much the same way as for the discrete systems). Thus for  $Q \leq \pi^2$  the functional is minimized by  $\mu \equiv 0$ . Moreover, similar reasoning shows that in this region, there is no non-trivial solution, formal or otherwise, to the Euler–Lagrange equation:

$$\mu'' + Q\mu(1 - \mu^2) = 0. \tag{4.19}$$

Thus the first half of the second item is proved.

Using the trial function  $\varepsilon \sin \pi x$ ;  $\varepsilon \ll 1$  it is seen that for  $Q > \pi^2$ ,  $\mathcal{F}_B(r)$  corresponds to non-trivial minimizers (or “near-minimizers”). Existence of a genuine minimizing solution will follow, actually, by quadrature, which ultimately proves the second half of the second statement.

Let us start by consideration of trial minimizers which, without loss of generality, are assumed to have piecewise continuous first derivative. The first observation is that in any such trial minimizer, the function may as well be symmetric with vanishing derivative at the mid-point. Symmetry follows immediately: If  $\mu$  is a trial function suppose, e.g., that

$$\int_0^{\frac{1}{2}} \mathcal{L}_Q(\mu) dx \leq \int_{\frac{1}{2}}^1 \mathcal{L}_Q(\mu) dx$$

then by replacing the right half of  $\mu$  with its reflection from the left, we get a trial function of caliber at least as good as  $\mu$ . Next, we show by similar means that in any trial function – symmetric or otherwise – the midpoint derivative may as well vanish (or the trial minimizer can be improved). For simplicity, we argue the symmetric case. Indeed, suppose that  $|\mu'(x)| \rightarrow \alpha > 0$  as  $x \rightarrow \frac{1}{2}$ . Let  $\varepsilon > 0$  denote a sufficiently

small number and let us consider the effect of replacing  $\mu(x)$  by  $\mu(\frac{1}{2} - \varepsilon)$  in the region  $\frac{1}{2} - \varepsilon \leq x \leq \frac{1}{2} + \varepsilon$ . It may be assumed that, for  $\varepsilon$  small, in this region,

$$c_1(\varepsilon)\alpha \leq \mu'(x) \leq c_2(\varepsilon)\alpha$$

with  $c_1, c_2 \rightarrow 1$  as  $\varepsilon \downarrow 0$ . Therefore, the benefit to the functional from cutting out the derivative term is at least, in absolute value,

$$\frac{1}{2}(c_1\alpha)^2 \cdot 2\varepsilon.$$

On the other hand, there will be “loss” to the functional because, presumably,  $\mu$  has been deprived of taking on optimal values in this region. Now the change in  $\mu$  between  $x = \frac{1}{2} - \varepsilon$  and  $x = \frac{1}{2}$  is at most  $c_2\alpha\varepsilon$ . If  $P_Q$  denotes the maximum value of the derivative of  $\frac{1}{2}Q\mu^2 - \frac{1}{4}Q\mu^4$ ,  $0 \leq \mu \leq 1$  it is seen that the loss is at most, in absolute value,

$$(P_Q c_2 \alpha \varepsilon) \cdot 2\varepsilon.$$

Clearly, for  $\varepsilon$  sufficiently small, the benefits outweigh the losses. Thus, under the *assumption* of a classical minimizer, we may presume that its derivative vanishes at the midpoint.

Now, the differential (Euler–Lagrange) equation equation displayed earlier admits the invariant

$$\frac{1}{2} \left( \frac{d\mu}{dx} \right)^2 + \frac{1}{2}Q\mu^2 - \frac{1}{4}Q\mu^4 = \text{const.}$$

On the basis of the preceding, we may identify the constant with value of the functional when the derivative vanishes:

$$\frac{1}{2} \left( \frac{d\mu}{dx} \right)^2 + \frac{1}{2}Q\mu^2 - \frac{1}{4}Q\mu^4 = \frac{1}{2}Q\mu_\ell^2 - \frac{1}{4}Q\mu_\ell^4$$

where  $\mu_\ell = \mu(\frac{1}{2})$ . It is noted, perhaps coincidentally, that the invariant of interest, namely  $-Q[\frac{1}{2}\mu_\ell^2 - \frac{1}{4}\mu_\ell^4]$  is the crucial item governing the rate that the free energy of the layer changes with the layer thickness.

In any case, we write the above

$$\left( \frac{d\mu}{dx} \right)^2 = Q(\mu_\ell^2 - \mu^2) \left[ 1 - \frac{1}{2}(\mu_\ell^2 + \mu^2) \right] \quad (4.20)$$

The preceding equation is actually true but trivial if  $Q \leq \pi^2$ . To avoid further provisos, let us assume for the midrange future that  $Q > \pi^2$  where by the trial function analysis discussed after Eq.(4.19), all quantities in Eq.(4.20) are non-trivial. (The relevant claims in the statement of this theorem at the point  $Q = \pi^2$  will follow, from both sides, by continuity.)

We now obtain an implicit expression for  $\mu$ , namely

$$\int_0^{\mu(x)} \frac{d\mu_\star}{(\mu_\ell^2 - \mu_\star^2)^{\frac{1}{2}} [1 - \frac{1}{2}(\mu_\ell^2 + \mu_\star^2)]^{\frac{1}{2}}} = \sqrt{Q}x, \quad (4.21)$$

$0 \leq x \leq \frac{1}{2}$ . And the above can be used to derive the following identity for  $\mu_\ell$ :

$$\int_0^{\mu_\ell} \frac{d\mu_\star}{(\mu_\ell^2 - \mu_\star^2)^{\frac{1}{2}} [1 - \frac{1}{2}(\mu_\ell^2 + \mu_\star^2)]^{\frac{1}{2}}} = \frac{1}{2}\sqrt{Q} : \quad (4.22)$$

These two equations (executed in reverse order) actually *define* the function  $\mu(x)$  as unfolds below. In particular, let us first show that the relationship in Eq.(4.22) defines a function  $\mu_\ell(Q)$  for  $Q \in [\pi^2, \infty)$  with values in  $[0, 1)$ .

To this end, It is convenient to rid the integral of the  $\mu_\ell$  dependence in the upper limit. We substitute

$$\mu = \mu_\ell \sin \theta$$

and Eq.(4.22) now reads

$$\int_0^{\frac{\pi}{2}} \frac{d\theta}{[1 - \frac{1}{2}\mu_\ell^2(1 + \sin^2 \theta)]^{\frac{1}{2}}} = \frac{1}{2}\sqrt{Q}. \quad (4.23)$$

This form manifestly defines the inverse function, the “forward” function  $\mu_\ell(Q)$  with the stated properties follows if we can demonstrate (strict) monotonicity and verify the ranges. These are immediate.

It is noted from Eq.(4.23) that  $\mu_\ell < 1$  implies  $Q < \infty$  with divergence of  $Q$  as  $\mu_\ell \uparrow 1$ . Moreover,  $\mu_\ell = 0$  certainly implies that  $Q = \pi^2$ . Finally, letting  $\mu_\ell^{(1)} > \mu_\ell^{(2)}$  – both in the specified range – it is seen by inspection that  $Q(\mu_\ell^{(1)}) > Q(\mu_\ell^{(2)})$ .

Thus far we have established the existence of  $\mu_\ell(Q)$  in  $[\pi^2, \infty)$  – which we may extend to “identically zero” in  $[0, \pi^2]$ . In the latter range,  $\mu(x)$  is just zero and in the former, it is given implicitly by Eq.(4.21). The remainder of item 2 and all of item 1 in the statement of this theorem has been proved. (Moreover, we now have some knowledge of the minimizing magnetization profile.)

We turn to item 3 which we establish by elementary asymptotic analysis of Eq.(4.23). Writing  $1 - \mu_\ell^2 = \varepsilon_Q$  and transforming  $\theta \rightarrow \frac{\pi}{2} - \phi$  we re-express Eq.(4.23):

$$\int_0^{\frac{\pi}{2}} \frac{d\phi}{(\varepsilon_Q + \frac{1}{2}(1 - \varepsilon_Q) \sin^2 \phi)^{\frac{1}{2}}} = \frac{1}{2} \sqrt{Q}. \quad (4.24)$$

Using  $q^2 = \frac{2\varepsilon_Q}{1-\varepsilon_Q}$ , the above amounts to

$$\int_0^{\frac{\pi}{2}} \frac{d\phi}{(q^2 + \sin^2 \phi)^{\frac{1}{2}}} = \left( \frac{2}{1 - \varepsilon_Q} \right)^{\frac{1}{2}} \frac{1}{2} \sqrt{Q} = \frac{1}{\mu_\ell} \sqrt{\frac{Q}{2}}. \quad (4.25)$$

Let  $\mathbb{I}_q$  denote the left side. We would like to replace the  $\sin^2 \phi$  with  $\phi^2$  – which certainly provides a lower bound:

$$\mathbb{I}_q \geq \int_0^{\frac{\pi}{2}} \frac{d\phi}{(q^2 + \phi^2)^{\frac{1}{2}}} = \sinh^{-1} \frac{\pi}{2q} \quad (4.26)$$

and which further implies the bound

$$1 - \mu_\ell \geq K_1 \exp - \left( \frac{Q}{2} \right)^{\frac{1}{2}} \quad (4.27)$$

with  $K_1$  a constant independent of  $Q$ . So, defining

$$\mathcal{E}_q = \mathbb{I}_q - \int_0^{\frac{\pi}{2}} \frac{d\phi}{(q^2 + \phi^2)^{\frac{1}{2}}} \quad (4.28)$$

we get an opposite bound of the form in Eq.(4.27) if we can show that  $\mathcal{E}_q$  is bounded by a constant of order unity independent of  $q$ . Subtracting out:

$$\mathcal{E}_q = \int_0^{\frac{\pi}{2}} \frac{\phi^2 - \sin^2 \phi}{(q^2 + \phi^2)^{\frac{1}{2}} (q^2 + \sin^2 \phi)^{\frac{1}{2}} [(q^2 + \phi^2)^{\frac{1}{2}} + (q^2 + \sin^2 \phi)^{\frac{1}{2}}]} d\phi. \quad (4.29)$$

In the numerator we may replace:

$$\phi^2 - \sin^2 \phi \leq \frac{1}{3} \phi^4 \quad (4.30)$$

and in the denominator, we may again replace  $\sin \phi$  with  $\phi$  and set  $q = 0$  with the result:

$$\mathcal{E}_q \leq \int_0^{\frac{\pi}{2}} \frac{\frac{1}{3} \phi^4}{2(\phi^2)^{\frac{3}{2}}} d\phi = \frac{1}{6} \int_0^{\frac{\pi}{2}} \phi d\phi \quad (4.31)$$

which establishes an opposite bound of the form in Eq.(4.27). All claims have been established.  $\square$

**Corollary 4.2** *The derivative of  $\mathcal{F}_B(r)$  with respect to  $r$  is, in fact given by the free energy function evaluated at the midpoint,  $\varphi_B(M_\ell(r, B))$ .*

*Proof.* Here, it is convenient to go back to the original form with unrescaled variables. We take from the above only the facts that (1)  $\mathcal{F}_B(r)$  can be differentiated in the first place, (2) that for all  $r$ , the minimizing  $M_B(x)$  has vanishing derivative at the midpoint and (3) the continuity of  $M_\ell(r, B)$ . Our proof consists of the continuum analog of Lemma 3.3. It may be assumed that  $Br^2 > A\pi^2$  otherwise, the desired result is trivial.

Using  $M_{r,B}(x)$  as temporary notation for the appropriate minimizing solution, consider first the situation on  $[0, r + \delta r]$ . As a trial function, we may use  $M_{r,B}(x)$  up to  $x = \frac{1}{2}r$  and then the constant  $M_{r,B}(\frac{r}{2}) (= M_\ell(r, B))$  in the region  $[\frac{r}{2} \leq x \leq \frac{r+\delta r}{2}]$  and, as for the right half, we reflect. The result is

$$\mathcal{F}_B(r + \delta r) \leq \mathcal{F}_B(r) + \delta r \varphi_B(M_\ell(r, B)) \quad (4.32)$$

and a one way bound has been established. On the other side, we can simply cut out the region  $[\frac{r}{2} \leq x \leq \frac{r+\delta r}{2}]$  (and its reflection) to obtain

$$\mathcal{F}_B(r) \leq \mathcal{F}_B(r + \delta r) - \int_{\frac{r-\delta r}{2}}^{\frac{r+\delta r}{2}} \left[ \frac{A}{2} M_{r+\delta r, B}^2 - \frac{B}{2} M_{r+\delta r, B} + \frac{U}{4} M_{r+\delta r, B}^4 \right] dx \quad (4.33)$$

By virtue of the fact that the derivative vanishes at the midpoint, the first term in the integral is  $o(\delta r)$ . As for what remains, we use continuity of  $M_{r+\delta r, B}$  as a function of  $x$  and continuity of  $M_\ell(r, B)$  as a function of  $r$  to obtain

$$\mathcal{F}_B(r) \leq \mathcal{F}_B(r + \delta r) - \delta r \varphi_B(M_\ell(r, B)) + o(\delta r) \quad (4.34)$$

which completes the proof.  $\square$

### 4.3 Evolution of thinning for strong wetting fluids

In this subsection, we commence investigation of the behavior of  $r_B$  for  $0 \leq B < \infty$ .

First off, we can no longer postpone a precise formulation of the of strong wetting condition. Mathematically, this condition is initially seen to be sufficient (but apparently not necessary) to insure that “something interesting happens” as the temperature parameter evolves. But it turns out – as will be demonstrated later – a

stronger condition along these lines is actually *required* to ensure that the layer does not dwindle away at low temperatures. (Discussion of various scenarios which can occur without the strong wetting condition are postponed to the next subsection.)

Under this criterion of strong wetting it will be readily demonstrated that the thinning process will inevitably experience discontinuities: either in  $r_B$  itself or (“generically unlikely”) in its derivative. Indeed the discontinuity will occur as soon as the current layer is *not* in the high temperature phase. Moreover, in the present context, the first such discontinuity necessarily implies that a turning point has been reached. Specifically: once  $r_B$  corresponds to a film thickness that is in the low temperature phase (or critical state) then, at least for a while thereafter,  $r_B$  is increasing.

These two points are not necessarily tied together and will be treated separately. In particular, the existence of the discontinuities appears to be quite robust. By contrast, the occurrence of thickening subsequent to non-trivial thermodynamic behavior in the layer is a direct consequence of the close ties between the physical descriptions of the bulk and layer problems. Indeed, if additional thermodynamic forces are incorporated into the layered system that are *not* present in the bulk, it might well be the case that thinning will continue after the discontinuities (as is apparently the case in the data from [8] and [7]).

We note that for temperatures just below the critical temperature (specifically,  $B > 0$  but less than  $A^{-1}\pi^2$ ) the layer is always subcritical and the thinning process follows an orderly evolution that we call *free thinning*. Here,  $r_B$  satisfies  $c(r_B) = -B^2/4U$ . Regardless of actual circumstances we shall denote the solution of the above by  $r_\circ$ :

$$r_\circ : c(r_\circ) = -\frac{1}{4} \frac{1}{U} B^2. \quad (4.35)$$

On the other hand, a layer of thickness  $r$  is in the low temperature phase provided  $r^2 B \geq A\pi^2$ . We define, for  $B > A\pi^2$ , the critical thickness  $r_\star$  as the exact thickness for a layer which, if present, is just entering the low temperature phase:

$$r_\star : Br_\star^2 = A\pi^2.$$

We formulate the condition of strong wetting in terms of these quantities:

**Definition 4.3** *Consider the continuum thinning problem as described. Then the system is said to satisfy the strong wetting condition if for some  $B$ ,*

$$r_\star(B) = r_\circ(B).$$

**Remark 4** We remark that the above does not require any coincidence of parameters and could be replaced by  $r_*(B) \leq r_o(B)$  for some  $B$ . Indeed  $r_o$  starts out “ahead” (meaning smaller) at  $B = A\pi^2$  and either  $r_*$  catches up at some point or it does not. Since both evolve continuously, the former implies the statement in the definition. It is noted that for any fixed  $c(r)$  as described, the system satisfies strong wetting provided  $U$  is sufficiently large and/or  $A$  is sufficiently small. Similarly, strong wetting is achieved if  $c$  is multiplied by a large “interaction strength” parameter.

On the other hand, a strong enough divergence of  $c(r)$  at  $r = 0$  implies strong wetting independent of these parameters. (Here, some small care must be taken to properly define the problem using cutoffs but these matters will not concern us for the present.) In particular, notwithstanding the appearance of the strong wetting construction, *some* condition along the lines of  $r_*(B) \leq r_o(B)$  for *all* values of  $B$  that are very large is, in fact, required in order for the continuum model to have sensible large  $B$  behavior. As previously promised, these matters will be discussed in the next subsection.

Interestingly enough, the critical potential for guaranteed strong wetting (and sensible large  $B$  behavior) is  $c(r) \sim r^{-4}$  namely the behavior associated with the mean-field  $-d \geq 4$  – Van der Waals interaction. Later we provide a sharp value for the coefficient which separates “sensible” from “nonsensible” large  $B$  behavior.

Since we have assumed  $c(r)$  is smooth and increasing this means that when  $r_B = r_o$  then  $r_B$  is smooth and decreasing. Our first result, which hardly requires a proof, is that the initial free thinning epoch extends somewhat beyond  $B = A\pi^2$

**Proposition 4.4** *Consider the continuum thinning problem as described in Eq.(4.16) and let*

$$B_T = \sup\{B \mid r_{B'} = r_o \text{ for all } B' < B\}.$$

*Then  $B_T = A\pi^2 + \vartheta$  for some  $\vartheta > 0$ .*

*Proof.* For ease of exposition, we will argue from the integrated form of all relevant quantities. We employ  $C(r)$  and  $\mathcal{F}_B(r)$  as defined and we recall  $r_B$  is the minimizer of  $C(r) + \mathcal{F}_B(r) - rf_B$ . For  $B \leq A\pi^2$ ,  $\mathcal{F}_B(r)$  vanishes identically and so, obviously  $r_B$  satisfies Eq.(4.35). Now consider  $B = A\pi^2 + \delta B$  with  $\delta B \ll 1$ . Then, as  $r$  varies, the only portion of  $C(r) + \mathcal{F}_B(r) - rf_B$  that is effected is the region  $1 \geq r \geq 1 - \delta r$  with  $\delta r \sim \frac{1}{2}\delta B/A\pi^2$  as  $\delta B \rightarrow 0$ . Under the assumption of strict monotonicity of  $c(r)$

and continuity of  $\mathcal{F}_B(r)$ , (which, anyway, scales like  $\delta B$ ) for  $\delta B$  sufficiently small, this region is well past the region of the minimum and not strong enough to dispute the free thinning candidate for  $r_B$  and the result follows.  $\square$

Of course the strong wetting condition ensures that the initial epoch of free thinning must eventually come to a close. Let us denote by  $r_\bullet$  the (largest) mutual value:

$$r_\bullet = \min\{r_\circ(B) \mid r_\circ \leq r_\star\} = \max\{r_\star(B) \mid r_\star \leq r_\circ\}.$$

Analysis of the circumstances under the purported condition  $r_B = r_\bullet$  lead, inevitably to the conclusion that there must be discontinuities.

**Theorem 4.5** *Consider the continuum thinning problem as described and suppose the system satisfies the strong wetting condition. Then the initial epoch of thinning is entirely the process of free thinning; i.e., the layer begins to re-thicken after  $B = B_T$ . Moreover, since  $r'_B < 0$  for  $B < B_T$  and  $r'_B \geq 0$  for  $B \gtrsim B_T$  there is always a discontinuity in the derivative at  $B = B_T$ . Moreover, at  $B = B_T$ , it is generic that  $r_B$  is discontinuous (with positive jump).*

*Proof of Theorem 4.5.* Let us entertain the possibility that the free thinning occurs till the layer thickness is down to  $r_\bullet$ . Denoting by  $B_\bullet$  the parameter value where this would occur, let us increase  $B : B_\bullet \rightarrow B_\bullet + \delta B$  which causes the change  $r : r_\bullet \rightarrow r_\bullet + \delta r$  with  $\delta B$ ,  $|\delta r| \ll 1$ . Then, to lowest order,  $\delta r$  and  $\delta B$  are related by

$$\left(c' + \frac{\partial \varphi_B(M_\ell)}{\partial r}\right) \delta r = \left(f'_B - \frac{\partial \varphi_B(M_\ell)}{\partial B}\right) \delta B \quad (4.36)$$

where all arguments are evaluated at  $(r_\bullet, B_\bullet)$ . The above formula must be taken *cum grano salis*; certainly it is valid if  $\delta r > 0$  but for  $\delta r < 0$  it is only true under the auspices that  $|\delta r|$  is not too large compared with  $\delta B$ . This fine point need not concern us since all relevant circumstances concerns the event that  $\delta r$  is positive.

This (first) claim is the following: regardless of the right side of Eq.(4.36), we claim that if coefficient of  $\delta r$  is negative, then at  $B = B_\bullet$ , the free energy is minimized at an  $r > r_\bullet$ . Indeed, supposing this quantity to be negative we would lower the free energy by simply increasing  $r$  above  $r_\bullet$ . Moreover, it is claimed that generically, either sign is possible. Since it turns out that this is not entirely obvious, a separate proposition to this effect will be provided immediately subsequent to the present proof. However, for

future reference, we remark that by this reasoning, whenever  $r = r_B$ , non-negativity of this quantity must follow:

$$c'(r_B) + \left[ \frac{\partial \varphi_B(M_\ell)}{\partial r} \right]_{(r_B, B)} \geq 0. \quad (4.37)$$

Back to the problem at hand, *negativity* of this combination at  $(r_\bullet, B_\bullet)$  implies that at  $B = B_\bullet$ , the free energy is minimized by an  $r_{B_\bullet} > r_\bullet$  which, in particular, implies a low temperature layer. Now, initially (e.g., as discussed in Proposition 4.4, for  $B \lesssim \pi^2 A$ ) the layer thickness,  $r_B (= r_o(B))$  corresponded to a high temperature layer under free thinning. By the time circumstances have permitted the opportunity to make the transition continuously through a critical layer it is apparently already in a low temperature layer. It follows that at the (existential) point  $B_T$  – which is evidently *less* than  $B_\bullet$  – there has been a discontinuous jump of the layer thickness. Indeed, at this point, there are coexisting minimizing layer thicknesses  $r_{B_T}^+ > r_{B_T}^-$  satisfying

$$\begin{aligned} [r_{B_T}^+]^2 B_T &> \pi^2 A && \text{(low temperature layer);} \\ [r_{B_T}^-]^2 B_T &< \pi^2 A && \text{(high temperature layer).} \end{aligned} \quad (4.38)$$

It is noted that the discontinuity must go backwards; in particular, by definition, up to and including  $(r_{B_T}^-, B_T)$ , the free thinning criterion is still satisfied.

In light of Proposition 4.6 below, these discontinuities are certainly generic. And needless to say, if the preceding negativity criterion fails, it might still be the case that at  $B = B_\bullet$ , the free energy is minimized at a larger value of  $r$  than  $r_\bullet$  due to a (sufficiently strong) turn around of  $c' + \frac{\partial \varphi_B}{\partial r}$  at  $r > r_\bullet$ ; the scenario for these cases is identical culminating in Eq.(4.38).

A number of interesting possibilities would ensue if the coefficient of  $\delta B$  in Eq.(4.36) were (“still”) negative. However, as will be demonstrated in Lemma 4.7, this quantity is positive. Thence, if  $c' + \frac{\partial \varphi_B}{\partial r}$  is also positive at  $(r_\bullet, B_\bullet)$  corresponding to an actual minimum of  $C(r) + F_B(r) - r f_B$  then  $r_B$  turns around and obviously does so with derivative going discontinuously from (strictly) negative to (strictly) positive.

Finally we turn to the case where  $c' + \frac{\partial \varphi_B}{\partial r}$  vanishes at  $(r_\bullet, B_\bullet)$ . Here one must look at higher order terms or, if necessary, non-perturbatively to ensure that  $C(r) + F_B(r) - r f_B$  is really uniquely minimized at  $r = r_\bullet$ . If not, there already has been a

jump in  $r_B$  or there is about to be a jump in  $r_B$ . If so, then in light of the positivity of  $f'_B - \frac{\partial \varphi_B}{\partial B}$  there will anyway be a turnaround of  $r_B$  with a sharp singularity in the derivative of  $r_B$  at  $B = B_\bullet^+$ .  $\square$

**Proposition 4.6** *Consider the functions  $c(r)$ ,  $r_\bullet(B)$ , etc., as defined. Then at the point  $r = r_\bullet$ ,  $B = B_\bullet$ , the quantity*

$$c'(r_\bullet) + \frac{\partial \varphi_B}{\partial r}(r_\bullet, B_\bullet)$$

*can be of either sign depending on the details of  $c(r)$ .*

**Remark 5** As the analysis below will show, the sign of the above displayed quantity depends only on the ratio of  $|r'_\star|$  to  $|r'_\circ|$  at  $r = r_\bullet$ . Since, it is recalled,  $r_\bullet$  is the *first* point of intersection of these curves, and  $r_\star$  is “coming from above”, it follows that  $|r'_\star(B_\bullet)| \geq |r'_\circ(B_\bullet)|$  (with equality only marginally possible). From a mathematical perspective, if any function  $r_\circ(B)$  is prescribed satisfying the constraints of monotonicity and the correct limiting behavior  $r_\circ(B) \rightarrow 1$  as  $B \rightarrow 0$  then the corresponding  $c(r)$  can be constructed. Indeed, denoting the inverse function of  $r_\circ(B)$  by  $B_\circ(r)$ , we may simply write

$$c(r) = -\frac{1}{4} \frac{B_\circ^2(r)}{U}.$$

Thus, assuming  $r_\circ(B)$  is smooth and (“first”) intersects  $r_\star$  at some point  $(r_\bullet, B_\bullet)$  then local distortions in the vicinity of this intersection point can achieve *any* ratio of  $|r'_\star|/|r'_\circ|$  in  $(1, \infty)$  with only mild effect on  $c(r)$ .

From a more physical perspective, suppose that  $r_\circ(B)$  – and hence  $c(r)$  – is immutable but we allow  $A$  as a control parameter. (While the condition of ferromagnetism puts bounds on the allowed values of  $A$  we shall ignore these fine points for the time being.) For ease of exposition, let us suppose we have a bounded derivative for  $r_\circ(B)$  at  $B = 0$  and, say,  $r_\circ(B)$  vanishes at  $B = H$  (e.g., the case of a linear potential). Then, as  $A \rightarrow 0$ ,  $B_\bullet \rightarrow 0$  and we will have  $|r'_\star(B_\bullet)|$  divergent. So, in particular, for  $A$  sufficiently small,  $|r'_\star(B_\bullet)| \gg |r'_\circ(B_\bullet)|$ . Note that in this range, there have to be multiple points of intersection between  $r_\star(B)$  and  $r_\circ(B)$  On the other hand, if  $A$  is large, we will find  $r_\star(B) > r_\circ(B)$  for all  $B$  in  $[0, H]$ . It follows that there is an  $A_c$  at which there a first point of intersection (and, generically, only a single point of intersection) at which the derivatives match.

*Proof of Proposition 4.6.* We write

$$|c(r_o)| = \frac{1}{4} \frac{B^2}{U}$$

and, differentiating, we have

$$|c'(r_o)| \left| \frac{dr_o}{dB} \right| = \frac{1}{2} \frac{B}{U} = |c(r_o)| \frac{2}{B}.$$

Thus, after just a few steps,

$$\left| \frac{dc}{dr} \right| \frac{r'_o}{r'_\star} |r'_\star| = 2 \frac{r_\star}{B} \left| \frac{c(r_\bullet)}{r_\bullet} \right|.$$

It is noted that the combination  $|r'_\star B / r_\star|$  amounts to a logarithmic derivative of  $r'_\star$  with respect to  $\log B$  and is exactly  $\frac{1}{2}$  so, evaluating at  $(r_\bullet, B_\bullet)$  we arrive at

$$|c'(r_\bullet)| = 4 \frac{r'_\star}{r'_o} \left| \frac{c(r_\bullet)}{r_\bullet} \right| \quad (4.39)$$

Now, let us turn attention to the free energetics. Writing

$$\varphi_B(M_\ell(r, B)) = -\frac{1}{2} \frac{B^2}{U} [\mu_\ell^2(Q) - \frac{1}{2} \mu_\ell^4(Q)] \quad (4.40)$$

(where  $Q = Br^2/A$ ) we have, in general,

$$\frac{\partial \varphi_B}{\partial r} = -\frac{1}{2} \frac{B^2}{U} (1 - \mu_\ell^2) \frac{d\mu_\ell^2}{dQ} \frac{\partial Q}{\partial r}$$

Now it is a direct consequence of Lemma 4.7 below that the quantity  $\mathbb{K}$  defined by

$$\mathbb{K} := \left. \frac{d\mu_\ell^2}{dQ} \right|_{Q_c} \quad (4.41)$$

satisfies  $\mathbb{K}Q_c \geq 1$ . (Here,  $Q_c = \pi^2$ .) However, as can be readily verified by perturbative calculations, the inequality is strict:  $1 < \mathbb{K}Q_c = \frac{\int_0^\pi \sin^2 \theta d\theta}{\int_0^\pi \sin^4 \theta d\theta} = \frac{4}{3}$ . Continuing the derivation we have

$$\left| \frac{\partial \varphi_B}{\partial r} \right|_{(r_\bullet, B_\bullet)} = \frac{1}{2} \frac{B^2}{U} \mathbb{K} \cdot 2rBA = 4 \left| \frac{c(r_\bullet)}{r_\bullet} \right| \mathbb{K}Q_c \quad (4.42)$$

which is strictly greater than (but comparable to) the quantity  $4|c(r_\bullet)|/r_\bullet$  which is the coefficient of  $r'_o(B_\bullet)/r'_\star(B_\bullet)$  that figures into the right hand side of Eq.(4.39). Thus, depending on the magnitude of  $r'_o(B_\bullet)$  to  $r'_\star(B_\bullet)$  the quantity in the display of the statement of this proposition can indeed be of either sign.  $\square$

The key inequality alluded to earlier (which demonstrates that after free thinning is over, thickening must commence – at least for a while) is now presented:

**Lemma 4.7** *Whenever  $r^2 B \geq A\pi^2$ ,*

$$\frac{\partial}{\partial B} \varphi_B(M_\ell(r, B)) < \frac{\partial}{\partial B} \varphi_B(M)$$

where, at  $r^2 B = A\pi^2$ , the derivative is interpreted as being in the positive direction.

*Proof.* As discussed previously, the inequality can be verified perturbatively for  $r^2 B - A\pi^2 \ll 1$ . Furthermore for large  $B$  (and fixed  $r$ ) this can be shown on the basis of asymptotics. As for the general case, writing  $M_\ell(r, B) = \mu_\ell M$  (with  $M^2 = B/U$ ) the object to be differentiated is

$$-\frac{B^2}{U} \left( \frac{1}{2} \mu_\ell^2 - \frac{1}{4} \mu_\ell^4 \right)$$

while on the right, it is just  $-\frac{1}{4} \frac{B^2}{U}$ . Multiplying through by  $\frac{1}{A} r^4$  which does not effect the *partial* derivative, the left side is, to within constants, the derivative w.r.t  $Q$  of  $Q^2 [\frac{1}{2} \mu_\ell^2 - \frac{1}{4} \mu_\ell^4]$  – which is to be compared with  $\frac{d}{dQ} \frac{1}{4} Q^2$ . Thus, it is enough to show that the derivative of  $Q^2(1 - \mu_\ell^2)^2$  is negative.

We go back to the implicit identity for  $\mu_\ell(Q)$ : Differentiating both sides of Eq.(4.23) w.r.t.  $Q$  yields the further identity

$$\int_0^{\frac{\pi}{2}} \frac{1 + \sin^2 \theta}{[1 - \frac{1}{2} \mu_\ell^2 (1 + \sin^2 \theta)]^{\frac{3}{2}}} d\theta \frac{d\mu_\ell^2}{dQ} = \frac{1}{\sqrt{Q}} \quad (4.43)$$

Now inside the integrand,

$$2 > 1 + \sin^2 \theta$$

and

$$\frac{1}{1 - \mu_\ell^2} > \frac{1}{[1 - \frac{1}{2} \mu_\ell^2 (1 + \sin^2 \theta)]}$$

so we arrive at

$$\frac{2}{1 - \mu_\ell^2} \int_0^{\frac{\pi}{2}} \frac{d\theta}{[1 - \frac{1}{2} \mu_\ell^2 (1 + \sin^2 \theta)]^{\frac{1}{2}}} \frac{d\mu_\ell^2}{dQ} \geq \frac{1}{\sqrt{Q}}. \quad (4.44)$$

Substituting from Eq.(4.23) we conclude

$$Q \frac{d\mu_\ell^2}{dQ} > (1 - \mu_\ell^2)$$

which is equivalent to the statement that  $\frac{d}{dQ} [Q(1 - \mu_\ell^2)]^2 < 0$ . □

## 4.4 Large $B$ asymptotics and strong wetting revisited

Once the discontinuity has occurred and the recovery of the layer has begun, we may begin to investigate the behavior at large  $B$ . Obviously if  $B \gg 1$ , then, for intermediate values of  $r$ ,  $M_\ell(r, B)$  is very close to  $M(B)$  and so derivative of  $\mathcal{D}_B(r)$  (c.f. the display prior to Theorem 4.1) is dominated by  $c(r)$  – which we have stipulated to be strictly negative. Thus, it would seem, we drive towards  $r = 1$ .

A calculation based on this display (prior to Theorem 4.1) along with the large  $Q$  asymptotics contained in Theorem 4.1 indicate that

$$r_B : c(r_B) \asymp -\frac{B^2}{U} \exp\left[-r\sqrt{\frac{2B}{A}}\right]$$

is anticipated. Thus, in particular if  $c(r) \asymp -(1-r)$  as  $r \rightarrow 1$ , then

$$r_B \asymp 1 - \frac{B^2}{U} \exp\left[-\sqrt{\frac{2B}{A}}\right].$$

It is remarked that in the above displays, the symbol  $\asymp$  implies the existence of upper and lower bounds of the indicated form (for sufficiently large  $B$ ) which may differ by numerical constants.

While the preceding is certainly “true” in some sense, we now arrive at a small embarrassment of the large  $L_0$ -theory. In particular, throughout this section, we have been attempting to minimize  $C(r) + \mathcal{F}_B(r) - r f_B$ . Our next initial claim is that unless this object is identically minus infinity (due to  $C(r) \equiv -\infty$ ) the layer will eventually disappear altogether. This is notwithstanding the fact that for reasonable models the above asymptotics will hold; evidently this is for large but not *too* large a value of the inverse temperature parameter  $B$ .

A proof of the statement concerning the disappearance of the layer will follow as an immediate corollary to the up and coming lemma. However, for the meanwhile, let us recall that for all intents and purposes  $C(r)$  is *defined* by

$$C(r) = \int_0^r c(s) ds$$

so in essence we are asking that the above integral be divergent at the lower limit (leading to the embarrassment:  $C(r) \equiv -\infty$ ).

Obviously the problem can be addressed by an elementary renormalization featuring a cutoff at the lower limit. However, even with this device, we shall later show

that, actually, a *sufficiently strong* divergence of  $c(r)$  is required in order to prevent destruction of the layer as  $B \rightarrow \infty$ .

We shall discuss these matters shortly after we show that the finite  $C(0)$  models indeed eventually dispense with their layers. The seminal result, which will be used throughout, concerns the existence of an asymptotic surface energy for the existence of a layer.

**Proposition 4.8** *For fixed  $r > 0$ , as  $B \rightarrow \infty$ ,*

$$\mathcal{F}_B(r) - rf_B \asymp \frac{A^{1/2}B^{3/2}}{U}.$$

*Further, the above holds even if  $r \rightarrow 0$  when  $B$  gets large provided that  $r^2B$  tends to infinity.*

*Proof.* Recalling the form of Eq.(4.18), let us seek asymptotics on

$$I_Q := \min_{\mu} \int_0^1 \mathcal{L}_Q(\mu) dx.$$

Note that the potential term, temporarily denoted by  $QV(\mu)$ , saturates at  $\mu = 1$  with value  $\frac{1}{4}Q$ . Working on  $[0, \frac{1}{2}]$ , we get an upper bound by using a trial function with linear rise to  $\mu = 1$  in the region  $[0, \Delta]$ . I.e.  $\tilde{\mu}(x) = \frac{x}{\Delta}$  in  $[0, \Delta]$  with  $\Delta$  to be determined; we will neglect any benefit from the potential portion of the functional in this region. As a result

$$\frac{1}{2}I_Q \leq \frac{1}{2} \frac{1}{\Delta^2} \times \Delta - \left(\frac{1}{2} - \Delta\right) \frac{1}{4}Q$$

I.e.,  $I_Q \leq -\frac{1}{4}Q + \frac{1}{\Delta} + \frac{1}{2}Q\Delta$ . It is noted that the first term represents the bulk free energy. The second term is positive and, minimizing over  $\Delta$ , we find

$$I_Q \leq -\frac{1}{4}Q + c_l \sqrt{Q}.$$

with  $c_l$  a constant of order unity.

We seek a complimentary upper bound. Recall that  $\mu(x)$  rises monotonically in  $[0, \frac{1}{2}]$  to its maximum value  $\mu_\ell(Q) < 1$ . For  $Q$  large,  $\mu_\ell$  is nearly one – certainly bigger than  $\frac{1}{2}$ . Let  $\Delta^*$  denote the point where  $\mu$  achieves  $\frac{1}{2}$ . Then

$$\frac{1}{2}I_Q \geq -\Delta^*QV\left(\frac{1}{2}\right) + \int_0^{\Delta^*} \frac{1}{2}(\mu')^2 dx - \left(\frac{1}{2} - \Delta^*\right) \cdot \frac{1}{4}Q.$$

I.e.,

$$I_Q \geq -\frac{1}{4}Q + \tilde{c}\Delta^*Q + \int_0^{\Delta^*} (\mu')^2 dx$$

with  $\tilde{c} > 0$  a positive constant of order unity.

Now, using Jensen's inequality,

$$\int_0^{\Delta^*} (\mu')^2 dx = \Delta^* \int_0^{\Delta^*} (\mu')^2 \frac{dx}{\Delta^*} \geq \Delta^* \left( \int_0^{\Delta^*} \mu' \frac{dx}{\Delta^*} \right)^2 = \frac{1}{\Delta^*} \left( \int_0^{\Delta^*} \mu' dx \right)^2 = \frac{1}{4} \frac{1}{\Delta^*}.$$

Thus we learn that  $I_Q \geq -\frac{1}{4}Q + \tilde{c}\Delta^* + \frac{1}{4}\frac{1}{\Delta^*}$ . This is true for the *actual*  $\Delta^*$  of the minimizer. It is thus certainly true that

$$I_Q \geq -\frac{1}{4}Q + \min_{\Delta} [\tilde{c}\Delta + \frac{1}{4}\frac{1}{\Delta}].$$

Minimizing, we obtain  $I_Q \geq -\frac{1}{4}Q + c_u\sqrt{Q}$ .

Now it is clear from Eq.(4.18) that

$$\mathcal{F}_B(r) - rf_B = \frac{AB}{rU} [I_Q + \frac{1}{4}Q]$$

with  $Q = r^2B/A$ . We thus have  $\mathcal{F}_B(r) - rf_B \asymp \frac{A^{1/2}B^{3/2}}{U}$  as promised; the only proviso being that the relevant  $Q$  go to infinity.  $\square$

On the basis of the preceding it is hard (from certain perspectives) to imagine anything besides a sharp constant in these relations. This is indeed the case – and will actually be needed later – but for those so inclined, such a result may simply be assumed and one may proceed directly to Corollary 4.10 below.

**Lemma 4.9** *There is a non-trivial  $\kappa$  (meaning  $0 < \kappa < \infty$ ) such that*

$$\lim_{Q \rightarrow \infty} [I_Q + \frac{1}{4}Q]Q^{-1/2} = \kappa.$$

*Equivalently if  $B \rightarrow \infty$  and  $r = r(B)$  (with  $r \leq 1$ ) is some function which ensures  $r^2B \rightarrow \infty$  as  $B \rightarrow \infty$  then*

$$[\mathcal{F}_B(r) - rf_B]B^{-3/2} \rightarrow \kappa$$

*as  $B \rightarrow \infty$ .*

*Proof.* Let  $r_1 = r_1(B)$  and  $r_2 = r_2(B)$  with  $r_1 < r_2$  be two functions that satisfy the above stated criterion. (As usual, these  $r$ 's may be thought of as fixed numbers but more flexibility is allowed and, actually, this sort of flexibility will be required later.) We denote the corresponding  $Q$ -values by  $Q_1$  and  $Q_2$  respectively. We may write

$$[\mathcal{F}_B(r_2) - r_2 f_B] - [\mathcal{F}_B(r_1) - r_1 f_B] = \int_{r_1}^{r_2} \frac{\partial}{\partial r} [\mathcal{F}_B(r) - r f_B] dr. \quad (4.45)$$

The argument of the integrand is known (c.f., Corollary 4.2) to be  $\varphi_B(M_\ell(r, B)) - f_B$ . We may express these quantities in terms of the dimensionless objects introduced in Theorem 4.1:  $M_\ell(r, B) = M(B)[\mu_\ell(Q)]$  and we have that (exactly)

$$\varphi_B(M_\ell(r, B)) - f_B = \frac{1}{4} \frac{B^2}{U} (1 - \mu_\ell^2(Q))^2 =: \frac{1}{4} \frac{B^2}{U} \varepsilon_Q.$$

Thus, so far,

$$[\mathcal{F}_B(r) - r f_B]_{r_1}^{r_2} = \frac{1}{4} \frac{B^2}{U} \int_{r_1}^{r_2} \varepsilon_Q dr$$

where  $[X(s)]_{s_1}^{s_2}$  is notation for  $X(s_2) - X(s_1)$ . We change the variable of integration to  $Q$ :  $dQ = 2A^{-1/2}B^{1/2}Q^{1/2}dr$ . Thus

$$\frac{1}{4} \frac{B^2}{U} \int_{r_1}^{r_2} \varepsilon_Q dr = \frac{A^{1/2}B^{3/2}}{8U} \int_{Q_1}^{Q_2} \frac{1}{Q^{1/2}} \varepsilon_Q dQ. \quad (4.46)$$

Since all associated  $Q$ 's are large, we may apply the asymptotics from Theorem 4.1, item (3):  $\varepsilon_Q \asymp e^{-\sqrt{2Q}}$ . The final integral is rapidly convergent with its principal contribution from the vicinity of the lower limit. We learn:

$$\lim_{B \rightarrow \infty} \frac{[\mathcal{F}_B(r_2) - r_2 f_B] - [\mathcal{F}_B(r_1) - r_1 f_B]}{B^{-3/2}} \leq \lim_{B \rightarrow \infty} \text{const.} \times \frac{A}{U} e^{-\sqrt{2Q_1}} = 0. \quad (4.47)$$

The combination of this result and the asymptotic statement of Proposition 4.8 (for the non-triviality clause) imply the second statement in this lemma.

As for the first statement, we write, once again,  $\mathcal{F}_B(r) - r f_B = \frac{AB}{rU} [I_Q + \frac{1}{4}Q]$ . Dividing both sides by  $\frac{B^{3/2}A^{1/2}}{U}$  we learn on the basis of our first result that

$$[I_Q + \frac{1}{4}Q]Q^{-1/2} \rightarrow \kappa$$

as  $Q \rightarrow \infty$ . □

**Corollary 4.10** If  $C(0) \neq -\infty$  then as  $B \rightarrow \infty$ ,  $r_B \rightarrow 0$ .

**Remark 6** If  $c(r)$  is a regular function, then  $C(0) \neq -\infty$  necessarily implies  $C(0) = 0$ ; notwithstanding, without any additional provisos, we may imagine a  $\delta$ -function at the origin with strength  $C_0$  (with  $C_0 < 0$ ) Thus,  $C(0^+) = C_0$  while  $C(0) = 0$ . In these circumstances, the stated result still holds and the proof is unaffected. However, depending on the regular part of  $C$ , in the presence of the  $\delta$ -functions the large  $B$  asymptotics may well be different – no matter how small  $C_0$ . More importantly, for large value of  $|C_0|$  – or a sizable “additive” value of  $C(r)$  for  $r \ll 1$  – sensible evolution of the layer towards  $r = 1$  will persist for correspondingly sizable values of  $B$ .

*Proof.* Consider the object to be minimized namely  $C(r) + \mathcal{F}_B(r) - r f_B$ . For  $r = 0$  (as opposed to  $0^+$ ) this is zero according to the present assumption. Supposing that

$$\limsup_{B \rightarrow \infty} = r_\infty > 0.$$

Let  $B_n \rightarrow \infty$  so as to satisfy  $r_n \rightarrow r_\infty$  where  $r_n := r_{B_n}$ . Then for  $n$  large,  $\frac{1}{A} r_n^2 B_n$  also gets large and the layer free energy satisfies

$$C(r_n) + \mathcal{F}_{B_n}(r_n) - r_n f_{B_n} \gtrsim C(r_\infty) + \kappa B_n^{3/2}$$

where  $\kappa > 0$  is discussed in Propositions 4.8 and Lemma 4.9. This is certainly bigger than zero for  $B$  sufficiently large (implying that  $r_B$  *must* converge to zero).  $\square$

**Remark 7** It is not hard to see that if  $|C(r)| < Kr$  for some finite  $K$  then for  $B$  sufficiently large,  $r_B$  will be identically zero. Indeed look along a sequence where  $r_B^2 B$  tends to some definite limit which could be finite or infinite. If the limit is infinite, then large  $Q$  asymptotics are applicable and we would have

$$C(r_B) + \mathcal{F}_B(r_B) - r_B f_B \approx -K r_B + \kappa B^{3/2}$$

so we would certainly be better off with zero. Alternatively, if  $r_B^2 B \rightarrow AQ$  with  $\pi^2 < Q < \infty$  then

$$\mathcal{F}_B(r_B) - r_B f_B \rightarrow \frac{AB}{rU} [I_Q + \frac{1}{4}Q]$$

(in the sense of ratios). The quantity in square brackets is strictly positive and as is seen, its coefficient is proportional to  $B^{3/2}$ ; again we are better off with zero. If

$r_B^2 B$  tends to zero the situation is not so clear in the  $Q$  language *but* if anyway  $r_B^2 B$  is eventually less than (or equal to)  $\pi^2$  then the layer term drops out of our analysis and  $C(r) - rf_B \geq [-K + \frac{1}{4}B^2/U]r$  and (for  $B$  large) we are again better off with zero.

By contrast, if  $\frac{1}{r}C(r)$  diverges as  $r \rightarrow 0$ , – which is merely the statement that  $c(r) \rightarrow -\infty$  – then for large  $B$  we are, at worst, back to free thinning with  $r_B = r_0$  as described in Eq.(4.35). Note that this includes the case of a  $\delta$ –singularity: Here, for  $r > 0$ ,  $C(r) = C_0 + C_\rho(r)$  (where  $C_\rho$  denotes the regular piece). Obviously the minimizer is to be found among the  $r > 0$  options since this is certainly less than  $-r\frac{1}{4}\frac{B^2}{U}$  for  $r$  small.

It is evident that systems with  $C(0^+) > -\infty$  – even those that heretofore have been demonstrated to have undergone thinning and substantive recovery in some reasonable interval of the parameter  $B$  – will ultimately undergo reentrant thinning behavior via another large discontinuity. And this can happen via termination of the layer (immediate or otherwise) at finite  $B$  or ultimate disappearance via a free thinning mechanism.

The distinction between the various modes of behavior which have been informally elucidated above is not all too important except as a mathematical curiosity: No effect of this sort seems to have been observed experimentally (to the authors’ knowledge) and, back in the discrete setting, such effects do not easily occur. Foremost, there is Proposition 3.2 which essentially guarantees that as  $\beta \rightarrow \infty$   $L_\beta$  *must* return to  $L_0$ . However, it is clear that the inequality  $|C_{L_0}| > J_1$  is inconsistent with the scaling in Eqs. (4.1) – (4.2).

Indeed, after a bit of reflection, it is seen that this scaling is tantamount to the assertion that

$$J_0, J_1 \gg V(a_0 L_0).$$

Thereafter – it is presumed – the minute changes in the free energy at  $\beta \gtrsim \beta_c$  ultimately augments the r.h.s. with an  $L_0^{-4}$  which “compensates” for the fact that  $V(a_0 L_0) \approx c(r=1)L_0^{-4}$  which in turn vindicates the extreme inequality in the above display. Thus, it must be accepted that the entirety of the large  $L_0$ –theory – which notwithstanding its shortcomings is reasonably satisfactory – also amounts to a theory for  $r$ ’s which do not deviate too much from unity. At smaller values of  $r$ , the theory (i.e., in form of the scaling of Eqs. (4.1) – (4.2)) breaks down. While this should not effect matters near  $r = 1$ , clearly it is required that some augmented scaling of the

attractive potential allows the behavior of  $V(x)$  at small scales to dominate  $B^{3/2}$  for  $B \gg 1$ .

The relevant cure obviously requires a non-integrable divergence of  $c(r)$  as  $r \rightarrow 0$  which in turn requires some formal adjustments to the theory. Let us tend to these preliminary matters.

We start by defining

$$C_{\varepsilon_0}(r) = \int_{\varepsilon_0}^r c(r') dr'$$

and

$$\mathcal{D}_B^{[\varepsilon_0]}(r) = C_{\varepsilon_0}(r) + \mathcal{F}_B(r) - r f_B.$$

Now it is clear that if  $\mathcal{D}_B^{[\varepsilon_0]}(r)$  is minimized by some  $r_B^{[\varepsilon_0]} > \varepsilon_0$  then for all  $\varepsilon < \varepsilon_0$ ,

$$r_B^{[\varepsilon]} = r_B^{[\varepsilon_0]}.$$

Moreover (for fixed  $B$ ) then for  $\varepsilon_0$  sufficiently small,  $r_B^{[\varepsilon_0]} > \varepsilon_0$ . Thus we may define the model via the small  $\varepsilon_0$  limit and, formally,

$$r_B = \lim_{\varepsilon_0 \rightarrow 0} r_B^{[\varepsilon_0]}.$$

Notwithstanding, a variant of Corollary 4.10 demonstrates that in fact the divergence of  $c$  must be sufficiently strong or else, as  $B \rightarrow \infty$ , the layer dwindles away as  $B \rightarrow \infty$ . The dividing line is precisely the mean-field version of the Van der Waals force which – coincidentally or otherwise – is related to the strong wetting condition.

**Definition 4.11** Recalling  $r_o$  ( $c(r_o) = -B^2/U$ ) and  $r_*$  ( $r_* = A^{1/2}\pi/\sqrt{B}$ ) and the strong wetting condition ( $r_* \geq r_o$ ) for *some*  $B$  we define

(i) An  $\eta$ -violation (of strong wetting) if for *all*  $B$  sufficiently large,

$$\eta r_*(B) > r_o(B).$$

(ii) An  $\eta$ -enhancement (of strong wetting) if for *all*  $B$  sufficiently large,

$$\eta r_*(B) < r_o(B).$$

As is easily demonstrated, these enhancements/violations correspond to (short distance) bounds by the mean-field Van der Waals attractive potential.

**Theorem 4.12** *Consider the continuum thinning problem as described in Eq.(4.16) but augmented with non-integrable  $c(r)$  as discussed prior to Definition 4.11. Then there is a number  $v \in (0, \infty)$  such that*

- *If  $c(r)$  has an  $\eta$ -violation with  $\eta < v$  then*

$$\lim_{B \rightarrow \infty} r_B = 0.$$

- *If  $c(r)$  has  $\eta$ -enhancement then with  $\eta > v$  then*

$$\lim_{B \rightarrow \infty} r_B = 1.$$

*Proof.* We claim that  $\eta$ -enhancements/violations are equivalent to Van der Waals bounds on  $c(r)$  for  $r$  small. Consider first the violations. We have, assuming  $B$  large enough,  $r_o < \eta r_\star$  so

$$-\frac{B^2}{U} = c(r_o) \leq c(\eta r_\star)$$

However  $\eta r_\star = \eta \sqrt{\frac{A}{B}} \pi$  so for all  $r$  sufficiently small,

$$-\frac{\eta^4 A^2 \pi^4}{U} \frac{1}{r^4} \leq c(r) \tag{4.48}$$

(which, if  $\eta$  is small, is seen to be a “weak” Van der Waals bound since both sides are negative). Similarly, for an enhancement, we get exactly the opposite bound as in Eq.(4.48) for  $r$  sufficiently small. In this vein, it is remarked that the proof of the two statements in this theorem are in essence identical after reversal of inequalities and we will not explicitly repeat the arguments; we focus on the  $\eta$ -violations.

Let us assume that

$$\limsup_{B \rightarrow \infty} = \tilde{r} > 0;$$

we shall demonstrate that (regardless of  $\tilde{r}$ ) this is impossible for  $\eta$  smaller than some  $v$  to be specified. Consider instead  $r = r(B)$  satisfying  $Br^2(B)/A = Q$  with  $Q$  any fixed number of order unity (an optimal value of which will be specified later). We will show that for  $\eta$  smaller than a particular value, we can produce a choice of  $Q$  for which  $C(\tilde{r}) + \mathcal{F}_B(\tilde{r}) - \tilde{r}f_B > C(r) + \mathcal{F}_B(r) - rf_B$  for  $B$  sufficiently large. (By continuity this demonstrates the stated result). First we write

$$C(\tilde{r}) - C(r) = \int_r^{\tilde{r}} c(r) dr + \int_{s_0}^{\tilde{r}} c(r) dr.$$

The second integral is a constant independent of  $B$  (and  $r$ ) and the first can be estimated via Eq.(4.48):

$$\int_r^{s_0} c(r)dr \geq -\frac{1}{3} \frac{\eta^4 A^2 \pi^4}{U} \frac{1}{r^3} + \text{const.}$$

Next we use the formula in Eqs.(4.45)–(4.46) to write

$$[\mathcal{F}_B(r') - r' f_B + C(r')]_{r'}^{\tilde{r}} \geq \frac{A^2}{U} \frac{1}{r^3} \left[ -\frac{1}{3}(\eta\pi)^4 + \frac{1}{8}Q^{3/2} \int_Q^{\tilde{Q}} \frac{1}{[Q']^{1/2}} \varepsilon_{Q'} dQ' \right] + \text{const.} \quad (4.49)$$

where  $\tilde{Q} = [\tilde{r}]^2 B/A$  and it is remarked that the integral formula is obviously valid even if  $Q < \pi^2$ . We may, of course, neglect consideration of the constant term since the principal term is multiplied by  $r^{-3} \rightarrow \infty$ . Similarly the upper limit on the integral may be replaced by infinity due to the rapid convergence of the integrand which easily absorbs the multiplicative singular term ( $\propto B^{3/2} \propto r^{-3}$ ). Consider, then, the quantity

$$\Gamma(Q) := \frac{1}{8}Q^{3/2} \int_Q^{\tilde{Q}} \frac{1}{[Q']^{1/2}} \varepsilon_{Q'} dQ'.$$

Obviously  $\Gamma(0) = 0$  and  $\Gamma(Q) \rightarrow 0$  (rapidly) as  $Q \rightarrow \infty$ . It therefore follows that there is a maximum to this function which is achieved at a finite (and non-zero) value  $Q = Q^\sharp$ . We denote this maximum value by  $\Gamma^\sharp$ ;  $0 < \Gamma^\sharp < \infty$ . Evidently if  $\frac{1}{3}(\eta\pi)^4 < \Gamma^\sharp$  and  $r^2 B/A = Q^\sharp$  the left hand side of Eq.(4.49) is positive and, therefore, the large  $B$ -minimum is near  $r = 0$  inversely proportional to  $B^{1/2}$ . We will call  $v$  the value of  $\eta$  which saturates the bound:

$$\frac{1}{3}\pi^4 v^4 = \Gamma^\sharp.$$

The argument under strong enhancement is quite similar. Supposing  $\liminf_{B \rightarrow \infty} r_B = 0$  we may again write our expression for  $Q$  assuming, if necessary along some sequence that the  $Q$ 's converge to some value. This value may be finite or infinite. Under  $\eta$ -enhancement, for any  $\tilde{r}$  of order unity, we obtain an inequality which is the exact reverse of Eq.(4.49) (with different constant terms). Now if we assume that  $\eta > v$ , the  $r = \tilde{r}$  behavior is more favorable, according to free energetics, than small  $r$  – regardless of the behavior of  $Q$ .

Finally we will show that if the superior limit of  $r_B$  is strictly positive then, in fact,  $r_B \rightarrow 1$ . Indeed the sharp asymptotics provided by Lemma 4.9 (c.f., Eq.(4.47)) indicate that for all sufficiently large  $B$ , the choice  $r = 1$  does better than any fixed  $r$  less than 1. Thence, on the basis of “derivatives” one recovers the asymptotics displayed at the beginning of this subsection.  $\square$

**Remark 8** It is noted that the mean-field Van der Waals attraction

$$c(r) = -\gamma \frac{1}{r^4}$$

is both enhancement and violation and is thus the borderline case. The theorem applies so evidently, there is a  $\gamma_c$  such that for  $\gamma < \gamma_c$  the layer disappears and for  $\gamma > \gamma_c$  it experiences full recovery.

Outside the realm of physics, it is therefore easy to construct models with strange behavior. Indeed, supposing  $c(r) = -\theta(r)\frac{1}{r^4}$  with  $\theta$  of order unity slowly varying above and below the critical value. Clearly, such potentials are capable of producing an infinite sequence of jumps back and forth between small minimizers and minimizers close to one.

## 5 Large $L_0$ mathematics

Our first result of this section will be a complete proof that the functional defined in Eq.(4.13) has a unique minimizer i.e., the one which we have produced by quadrature. (Here it will be convenient to work with the dimensionless version). Since it may be assumed that results along these lines are well established, we will be as succinct as possible. Moreover, several of the principal steps have already been established in the context of and Theorem 4.1 and Corollary 4.2

**Theorem 5.1** *Consider the functional*

$$\mathcal{F}_Q(\mu) := \int_0^1 \mathcal{L}_Q(\mu) dx \quad \left( = \int_0^1 \left[ \frac{1}{2} \mu'^2 - Q \frac{1}{2} \mu^2 + Q \frac{1}{4} \mu^4 \right] dx. \right)$$

*Then  $\mathcal{F}_Q$  has the unique minimizer which is identically zero for  $Q \leq \pi^2$  and given by the implicit formulas provided in Eq.(4.21) and Eq.(4.22) for  $Q > \pi^2$ .*

*Proof.* The situation for  $Q \leq \pi^2$  has been discussed; let us assume that  $Q > \pi^2$ . We start by considering a minimizing sequence  $(\mu_{[k]} \mid k \in \mathbb{N})$  for the functional  $\mathcal{F}_Q$  which, as previously mentioned, we may consider to be piecewise smooth. Since all quantities are even, we may only consider elements that do not change sign, without loss of generality non-negative. Since the “potential” term namely  $-\frac{Q}{2}\mu^2 + \frac{Q}{4}\mu^4$  is bounded below with bound saturating at  $\mu = 1$ , it may be assumed that for all  $k$ ,  $0 \leq \mu_{[k]}(x) \leq 1$ . Since the potential term is finite, the “kinetic” term must be separately finite, i.e., for each  $\mu_{[k]}$  in the sequence,  $\int (\mu'_{[k]})^2 dx$  is bounded by a constant independent of  $k$ . Thus,  $(\mu_{[k]})$  is a bounded sequence in  $H_0^1[0, 1]$ . We let  $\mu$  denote the weak limit. By employing trial functions (e.g.,  $\varepsilon \sin \pi x$ ;  $\varepsilon \ll 1$  as discussed shortly after Eq.(4.19)) we know that the limiting  $\mu$  is non-trivial. We will show that  $\mu$  is actually a minimizer for  $\mathcal{F}_Q(\cdot)$ . First, by weakness of the convergence (AKA lower semicontinuity)

$$\lim_{k \rightarrow \infty} \int_0^1 (\mu'_{[k]})^2 dx \geq \int_0^1 (\mu')^2 dx.$$

Further, by Sobolev embedding,  $\int \mu_{[k]}^2 dx \rightarrow \int \mu^2 dx$  and, by boundedness, a similar result applies for the fourth power. Thus, indeed,  $\mu$  is a genuine minimizer for the functional. Our aim is to show that this  $\mu$  is none other than the classical  $\mu_Q$ .

We may look to the weak form of the Euler–Lagrange equation which here implies that for any suitable test function  $\eta$ , the quantity

$$\mu' \eta' - Q(\mu - \mu^3) \eta$$

integrates to zero. This necessarily implies that  $\mu'$  itself has a weak derivative (namely  $+Q(\mu - \mu^3)$ ) which places  $\mu$  in a higher Sobolev space, e.g.  $W^{2,\infty}[0, 1]$ . But now since  $\mu' \in W^{1,\infty}[0, 1]$  the weak derivative of  $(\mu')^2$  exists and is given by  $2\mu' \times$ [the weak derivative of  $\mu'$ ]. Thus, in conclusion, the quantity

$$\frac{1}{2}(\mu')^2 + Q\left(\frac{1}{2}\mu^2 - \frac{1}{4}\mu^4\right)$$

has zero weak derivative i.e., is a.e. constant. We can now establish, essentially by the classical arguments employed in Theorem 4.1 that  $\mu'$  vanishes at (and is small in the neighborhood of)  $x = \frac{1}{2}$ . Indeed, suppose that in some very small neighborhood of  $x_\varepsilon := \frac{1}{2} - \varepsilon$ , the function  $\mu'$  averages to  $H\varepsilon$  with  $H$  large to be specified below. Then since the weak derivative of  $\mu'$  is bounded above (by  $Q$ ) we may conclude that

throughout  $(x_\varepsilon, \frac{1}{2})$   $\mu'$  is bounded above by  $H_1\varepsilon$  and below by  $H_2\varepsilon$  where  $H_1$  and  $H_2$  are large numbers comperable to  $H$ .

We will consider an alternative to  $\mu$  which we denote by  $\tilde{\mu}$ . Here (restricting attention to the left half of  $[0, 1]$  and reflecting) we define  $\tilde{\mu} = \mu$  for  $x < x_\varepsilon$  and  $\tilde{\mu} \equiv \mu(x_\varepsilon)$  in  $[x_\varepsilon, \frac{1}{2}]$ . We now show that if  $H$  is to large,  $\tilde{\mu}$  would provide a better minimizer for the functional than  $\mu$ . Indeed, the “gain” from the kinetic (derivative) portion of the functional is at least  $H_2^2\varepsilon^2 \times \varepsilon$ . As for the “potential” portion of the functional, Let us write, for  $x \in (x_\varepsilon, \frac{1}{2})$ ,

$$\mu(x) = \mu(x_\varepsilon) + \delta\mu(x).$$

Then for all such  $x$ ,  $\delta\mu$  is bounded above by  $\varepsilon^2 H_1$ . Now, the derivative with respect to argument of the potential term – i.e.,  $-\frac{Q}{2}\mu^2 + \frac{Q}{4}\mu^4$  which we temporarily denote by  $V(\mu)$  – is always smaller in magnitude than  $\frac{1}{2}Q$ . Thence in  $(x_\varepsilon, \frac{1}{2})$ ,

$$|V(\mu) - V(\tilde{\mu})| = |V(\mu(x_\varepsilon) + \delta\mu) - V(\mu(x_\varepsilon))| \leq \frac{1}{2}Q\varepsilon^2 H_1.$$

Thus the potential loss is no more than  $\frac{1}{2}Q\varepsilon^3 H_1$  which is much smaller than  $H_2^2\varepsilon^3$  if  $H$  is large. Thus, evidently for some mild value of  $c$  we must have  $|\mu'(x)| < c|\frac{1}{2} - x|$  for a.e.  $x$ . In particular, the derivative “vanishes” (e.g., in the sense of the Lebesgue average) at  $x = \frac{1}{2}$ . We may identify the a.e. constant value of  $\frac{1}{2}(\mu')^2 + Q(\frac{1}{2}\mu^2 - \frac{1}{4}\mu^4)$  with the value of  $Q(\frac{1}{2}\mu^2 - \frac{1}{4}\mu^4)$  at the midpoint. In particular then Eq.(4.20) indeed holds a.e. on  $[0, 1]$ . The production of the unique classical solution now follows the derivations in Eq.(4.21) and Eq.(4.22) and we have established that our minimizer is the (classical)  $\mu_Q$ .  $\square$

**Proposition 5.2** *Let  $m_k^{[L]} = m_k^{[L]}(\beta)$  denote the solution to Eq.(4.10) for  $1 \leq k \leq L$  where  $L = [rL_0]$  with  $L_0$  serving to define the temperature parameter  $B$  and  $r \in [0, 1]$  fixed. We define for  $x \in [0, 1]$  of the form  $x(L+1) = \text{integer}$ ,*

$$M_{r^2 B}^{[L]}(x) := Lm_{x(L+1)}^{[L]}(\beta)$$

*where the relation between  $\beta$  and  $B$  is given in Eq.(4.3). For general  $x \in [0, 1]$  we define  $M_B^{[L]}(x)$  via linear interpolation. Then, for any  $p < \infty$ ,  $M_{r^2 B}^{[L]}(x)$  converges strongly in  $W^{1,p}$  to the unique non-trivial (if applicable) function associated with  $\mathcal{F}_Q$  (as described in Eq.(4.17)).*

*Proof.* We start with the observation (from Theorem 2.1 item 4) that for every  $x$  and  $B$ ,  $M_B^{[L]}(x)$  is essentially bounded by  $M(B)$  ( $= \sqrt{3B}$ ), i.e., for any  $\lambda > 1$ ,

$$M_B^{[L]}(x) < \lambda M(B)$$

for all  $L$  sufficiently large. Thus  $(M_B^{[L]}(x))$  is a sequence of bounded functions on  $[0, 1]$  and we may extract a subsequence which converges, weakly e.g., in  $L^2[0, 1]$ . We will denote the weak limit by  $M_B^*(x)$ ; our aim is to show that this  $M_B^*(x)$  is  $M_B(x)$ , the solution to Eq.(4.12), whose properties were elucidated in Theorem 4.1.

To this end, we note that Eq.(4.12) is in fact satisfied *in weak form* by  $M_B^*(x)$ . Let  $\eta(x)$  denote an infinitely differentiable function on  $[-\varepsilon, 1 + \varepsilon]$  for some small  $\varepsilon$  and, for appropriate integer  $k$ , let  $\eta_k := \eta(\frac{k}{L})$ . Then, multiplying Eq.(4.10) by  $\eta_k$  and summing we have (with the superscript  $[L]$  suppressed)

$$\sum_{k=0}^{L+1} a\eta_k \Delta m_k = \sum_{k=0}^{L+1} (\text{Arctanh}(m_k) - bm_k)\eta_k. \quad (5.1)$$

We may sum by parts:

$$\sum_{k=0}^{L+1} a\eta_k \Delta m_k = \sum_{k=0}^{L+1} am_k \Delta \eta_k$$

(where we have used that  $m_k$  is identically zero outside  $\mathbb{L}$ ). Now, multiplying by  $L^3$  and replacing sums by integrals (which only procures an error that vanishes as  $L \rightarrow \infty$ )

$$\int_0^1 AM_B^{[L]}(x)\eta''(x)dx = \int_0^1 (-BM_B^{[L]}(x) + \frac{1}{3}(M_B^{[L]})^3)\eta(x)dx + o(\frac{1}{L}) \quad (5.2)$$

where the error term also accounts for the expansion of the arctangent. Now the above equation does not *immediately* imply that the weak form of Eq.(4.12) is satisfied by the limiting  $M_B^{[L]}(x)$  because we have no guarantee of the convergence (weak or otherwise) of  $(M_B^{[L]})^3$ . For this reason *and* in order to be able to identify the limit, we shall seek bounds on the gradients of the  $m_k$ . (We remark that the former motivation can be satiated by somewhat easier means than the forthcoming but we must still handle the latter.) We shall argue somewhat informally since a similar derivation has already been presented in the context of the continuum model. In the forthcoming, while we will be working on the lattice –  $L$  still finite, we will rescale  $\mathbb{L}$  to the unit

interval. Thus e.g., when we speak of the  $\varepsilon$ -neighborhood of the midpoint, we are actually describing the order of  $\varepsilon L$  sites.

We claim a linear bound on  $\nabla m_k^{[L]}$  in the direction away from the midpoint. Specifically for  $s \in (0, \frac{1}{2})$  there is a finite  $\mathbb{H} = \mathbb{H}(a, b)$  such that for all  $L$  sufficiently large,

$$\nabla m_{k_s}^{[L]} < \mathbb{H} s m_b \frac{1}{L}$$

where  $k_s$  is the closest point further than  $Ls$  lattice sites from the midpoint and, we remind the reader  $m_b$  is the bulk magnetization.

Suppose, then that this is violated: I.e., for a large  $\mathbb{H}$  – the specifics of which will be clarified below – the above is an equality for some  $s \in (0, \frac{1}{2})$ . Now on account of Theorem 2.2 item (ii) (that the Laplacian is negative) this actually represents an upper bound on the magnitude of the gradient in the  $s$ -neighborhood of the midpoint. Our first contention is that at the midpoint (and therefore throughout the neighborhood) the derivative will *still* be of this order if  $\mathbb{H} \gg B$ . Indeed for  $k, k'$  in  $\mathbb{L}$ , we may use the mean-field equation (Eq.(2.4)) to obtain

$$|\nabla m_k^{[L]} - \nabla m_{k'}^{[L]}| \leq \frac{1}{a} \sum_{j=k}^{j=k'} |\text{Arctanh}(m_j^{[L]}) - b m_j^{[L]}| \quad (5.3)$$

Now each  $m_j^{[L]}$  is less than  $m_b$  (by Theorem 2.1 item (4)) so  $b m_j^{[L]} \geq \text{Arctanh}(m_j^{[L]})$  and thus  $b m_j^{[L]} - \text{Arctanh}(m_j^{[L]}) \leq (b-1)m_j^{[L]} \leq (b-1)m_b$ . Thus for  $k - k' \leq sL$  the most the derivative could fall is  $(b-1)m_b s L = B m_b s L^{-1}$  so now (assuming  $B \ll \mathbb{H}$ ) we have that at the midpoint (and throughout the  $s$ -neighborhood)

$$|\nabla m_\ell^{[L]}| \geq \frac{\mathbb{H}' s m_b}{L} \quad (5.4)$$

with a complimentary upper bound.

We shall first show that this is impossible (for  $\mathbb{H}$  too large) on the basis of free energetics. Indeed, considering a “small”  $\varepsilon$ -neighborhood of the midpoint, it is seen that by replacing the ostensibly minimizing magnetization profile with its value at  $k_\varepsilon$  throughout this neighborhood, there is a lowering of the “kinetic” portion of the free energy at least as large as

$$\mathbb{H}_1^2 \varepsilon^2 m_b^2 \frac{1}{L^2} \times 2\varepsilon L \sim \frac{\mathbb{H}^2 \varepsilon^3 m_b^2}{L}$$

The calculation for the “potential” term is surprisingly similar. Let us write, for  $k_\varepsilon \leq k \leq \ell$ , the magnetization as  $m_k = m_{k_\varepsilon} + \delta m_k$  where, for convenience, we have temporarily dropped the  $[L]$  superscript. Then, according to the gradient upper bound,

$$\delta m_k \leq \frac{\mathbb{H}\varepsilon m_b}{L} \cdot \varepsilon L = \mathbb{H}\varepsilon^2 m_b. \quad (5.5)$$

Now the potential term in the discrete free energy functional is simply  $-\frac{1}{2}bm_k^2 - S_I(m_k)$  which is temporarily denoted by  $\Omega_b(m_k)$ . Then, for each  $k$  in the  $\varepsilon$ -neighborhood of the midpoint, the raise in the free energy after the truncation at  $k = k_\varepsilon$  is no more than

$$\max_{0 \leq m \leq m_b} [\Omega'_b(m)] \delta m_k \leq \max_{0 \leq m \leq m_b} [\Omega'_b(m)] \mathbb{H}\varepsilon^2 m_b.$$

But  $\Omega'_b(m)$  is exactly  $bm - \text{Arctanh}(m)$  which, in the range of interest is not more than  $(b-1)m_b$ . Thus the potential loss is no more, in magnitude, than

$$\mathbb{H}\varepsilon^2 m_b \cdot (b-1)m_b \cdot 2\varepsilon L \sim \frac{\mathbb{H}\varepsilon^3 m_b^2}{L}$$

By (informal) comparison with the “kinetic benefit” a few displays above, it is clear that  $\mathbb{H}$  cannot be too large; and, in addition there must be an actual linear bound (with a not too large  $H$ ) on  $\nabla m_k^{[L]}$  of the form in the display just before Eq.(5.3).

Recalling that  $M_B^{[L]}(x)$  was defined by linear interpolation, this means that the (weak) derivative,  $(M_B^{[L]})'(x)$  – which is piecewise constant – is essentially bounded. Thus, going to a further subsequence if necessary, it may be assumed that  $(M_B^{[L]})$  is converging to  $M_B^{[L]}$  weakly in  $W^{1,p}$  for any finite  $p$ . Whence (again by the Sobolev embedding theorem)  $M_B^{[L]}$  itself converges strongly in  $L^p$  and the weak version of Eq.(4.12) is indeed satisfied by  $M_B^*(x)$ .

In the context of Theorem 5.1, we know that for  $r^2 B \leq A\pi^2$  the only solution is  $M_B \equiv 0$ ; here we are fine. For  $r^2 B > A\pi^2$ , weak solutions include the unique non-trivial minimizer associated with the functional  $\mathcal{F}_Q$  as well as the trivial solution. We must rule out the latter. This is accomplished by invoking Proposition 2.4 which, in the current language bounds  $M_B^{[L]}(x = \frac{1}{2})$  below strictly away from zero uniformly in  $L$  for all  $L$  sufficiently large (whenever  $B > A\pi^2$ ). This midpoint bound together with the (uniform) bound on the weak derivative establishes that  $M_B^*(x)$  indeed corresponds to the non-trivial solution in the regime  $B > A\pi^2$ .

Finally, we refer back to Eq.(5.2) which, along with the uniform bound (below by zero and above by  $M(B)$ ) on  $M_B^{[L]}(x)$  implies the existence of a bounded (weak)

second derivative. Thus, the weak convergence can be promoted to the space  $W^{2,p}$  which implies strong convergence in  $W^{1,p}$   $\square$

**Corollary 5.3**  $\mathcal{F}_B(r)$  is given by

$$\mathcal{F}_B(r) = \lim_{L_0 \rightarrow \infty} L_0^3 F_{[rL_0]}. \quad (5.6)$$

Moreover

$$\lim_{L_0 \rightarrow \infty} \frac{L_\beta}{L_0} = r_B$$

*Proof.* The object  $L_0^3 F_L$  is, in accord with Eq.(5.2) the appropriate free energy functional for the continuum model “evaluated at”  $M_B^{[L]}(x)$ . (It is emphasized that the error terms involve expansions of the entropy term and do *not* involve gradients of  $M_B^{[L]}(x)$ . Thus, with the uniform bounds on  $M_B^{[L]}(x)$  these disappear in the large  $L_0$  without need for further discussion.) Using the strong  $W^{1,p}$  convergence of  $M_B^{[L]}(x)$  to the minimizer of the appropriate continuum free energy functional, the first result follows.

The second item follows from the first: If it is imagined (e.g., along a subsequence) that  $L_\beta/L_0$  is converging to something other than  $r_B$  then, on the basis of the above,  $L_\beta$  would not minimize  $\mathbb{D}_L$  – associated with the  $L_0$  model – for  $L_0$  sufficiently large.  $\square$

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