SLOWLY-MIGRATING TRANSITION LAYERS FOR THE DISCRETE ALLEN-CAHN AND CAHN-HILLIARD EQUATIONS

CHRISTOPHER P. GRANT* AND ERIK S. VAN VLECK†

Abstract. It has recently been proposed that spatially discretized versions of the Allen-Cahn and Cahn-Hilliard equations for modeling phase transitions have certain theoretical and phenomenological advantages over their continuous counterparts. This paper deals with one-dimensional discretizations and examines the extent to which dynamical metastability, which manifests itself in the original partial differential equations in the form of solutions with slowly-moving transition layers, is also present for the discrete equations. It is shown that, in fact, there are transition-layer solutions that evolve at a speed bounded by $C_1\varepsilon(1 + C_2/(n\varepsilon))^{-C_3n+C_4}$ for all $n \geq n_0$ and $\varepsilon \leq \varepsilon_0$, where $1/n$ is the spatial mesh size, ε is the interaction length, and n_0 and ε_0 are constants.

Key words. Cahn-Hilliard equation, Allen-Cahn equation, lattice differential equations, metastability

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Abbreviated title. Slowly-Migrating Transition Layers

1. Introduction. Two important partial differential equations for modeling the formation and motion of phase boundaries are the Allen-Cahn equation [4]

$$(1.1) \quad \begin{aligned} u_t &= \varepsilon^2 \Delta u - f(u), & x \in \Omega \\ \partial_\nu u &= 0, & x \in \partial\Omega, \end{aligned}$$

and the Cahn-Hilliard equation [11], [13]

$$(1.2) \quad \begin{aligned} u_t &= -\Delta(\varepsilon^2 \Delta u - f(u)), & x \in \Omega \\ \partial_\nu u &= \partial_\nu \Delta u = 0, & x \in \partial\Omega. \end{aligned}$$

In both equations, Ω is a bounded domain, ε is a small positive constant called the *interaction length*, and $f(u)$ is the derivative of a potential function $W(u)$ that has two wells of equal depth. For concreteness and simplicity, we will assume that $W(u) = (u^2 - 1)^2/4$, but results similar to those obtained in this paper may be obtained for qualitatively similar W .

In this paper, we will study the following systems of ordinary differential equations that are obtained by spatially discretizing (1.1) and (1.2) when $\Omega = (0, 1)$:

$$(1.3) \quad \begin{aligned} \dot{u}_i &= \nu^2(u_{i-1} - 2u_i + u_{i+1}) - f(u_i), & i = 0, \dots, n \\ u_{-1} &= u_0, u_n = u_{n+1} \end{aligned}$$

and

$$(1.4) \quad \begin{aligned} \dot{u}_i &= -n^2(\mu_{i-1} - 2\mu_i + \mu_{i+1}), & i = 0, \dots, n \\ u_{-1} &= u_0, u_n = u_{n+1} \\ \mu_i &= \nu^2(u_{i-1} - 2u_i + u_{i+1}) - f(u_i), & i = 0 \dots n \\ \mu_{-1} &= \mu_0, \mu_n = \mu_{n+1}. \end{aligned}$$

* Department of Mathematics, Brigham Young University, Provo, Utah 84602 USA.

† Department of Mathematical and Computer Sciences, Colorado School of Mines, Golden, Colorado 80401 USA. The work of this author was supported in part by NIST grant # 60NANB4D1698.

Here, each u_i is a function of the time t , and “ $\cdot$ ” represents differentiation with respect to t . Also, $1/n$ is the spacing between meshpoints, and $\nu = n\varepsilon$. Although we consider the discrete analog of Neumann boundary conditions in (1.3) and (1.4), similar results may be obtained for other boundary conditions.

The particular phenomenon we wish to address here is the slow migration of phase boundaries. For both (1.1) and (1.2), solutions corresponding to small inhomogeneous perturbations from $u = 0$ will typically develop sharp transition layers separating regions where u is close to -1 from regions where u is close to $+1$ (see, *e.g.*, [15], [19], [27]). Subsequently, these layers slowly migrate. When Ω is one-dimensional the layers move at a speed that is $O(e^{-C/\varepsilon})$ as $\varepsilon \rightarrow 0$, where C depends only on the distance between layers [1], [5], [14], [25], [26], [28]. For higher-dimensional Ω , the speed of migration remains exponentially small for (1.2) if the interfaces are nearly circular [2], [3], but is only $O(\varepsilon^2)$ for (1.1) because motion is then driven by curvature [9], [15], [18], [24], [31]. These slowly-moving solutions are interesting because, although far from any true equilibrium state, they may easily be mistaken for such. This behavior is called *dynamical metastability* by Bronsard and Kohn [8] and *dormant instability* by Fusco and Hale [26].

It is natural to ask to what extent slow motion is preserved when the space variable is discretized. The following results are known:

1. For ε fixed, as $n \rightarrow \infty$, the speed of transition layers (on finite time intervals) becomes asymptotically of order $e^{-C/\varepsilon}$ (see [23]).
2. For n fixed, if ε is sufficiently small then any transition-layer state is close to a (true) stable equilibrium, so no significant motion occurs (on *any* time scale) (see [22], [29]).

Our contribution is to show that the slowness of the motion in equations (1.3) and (1.4) can be estimated in terms of ε and n , within certain (independent) bounds on those parameters. Our results do not depend on the available results for the corresponding PDEs, but we have made use of techniques which were originally invented to handle PDEs but which we have been able to interpret abstractly in a way that makes them applicable to the discrete equations directly.

We have chosen to study these discrete equations for several reasons. The first reason is that the equations represent a simple scheme that might be used to simulate (1.1) and (1.2) numerically. (However, we make no attempt to match the slowness of the motion for (1.3) and (1.4) to that for (1.1) and (1.2).) The second reason is that these spatially discrete equations often exhibit extremely robust phenomena that are not present in the corresponding PDEs (see for example [12]). Third, they are of theoretical interest in their own right because the physical phenomena being studied are actually particulate in nature; indeed, the partial differential equations are often derived as continuum approximations of discrete systems (see [10], [17] and [30] for examples in the material sciences).

In the biological sciences, equations of the form (1.3) on an infinite lattice have been proposed as a model for propagation of nerve pulses in myelinated axons and have been addressed by several authors [6], [7], [16], [32], [35], [36], and [37]. In particular, the existence and stability of traveling wavefronts have been studied for a nonsymmetric double well potential W . Although the mechanisms driving wavefronts on finite and infinite lattices seem fundamentally different, there is the following connection between the two cases: Using summation by parts, it can be shown that when W satisfies the equal-well condition we required, any wavefront is, in fact, stationary, and a truncation of such a stationary wave is utilized in Section 4 of the present paper.

In order that our results may be stated precisely, we introduce some notation and

terminology. Given a continuous function $u : [0, 1] \rightarrow \mathbf{R}$, let $Z(u)$ be the set of zeros of u ; if u is an element of the $(n + 1)$ -dimensional vector space of real column vectors

$$U_n = \{(u_0, u_1, \dots, u_{n-1}, u_n)^T : u_i \in \mathbf{R}\},$$

let $Z(u)$ be the set of zeros of the piecewise linear interpolation of the data $\{(i/n, u_i) : i = 0, \dots, n\}$. Let $d(\cdot, \cdot)$ be the Hausdorff distance between sets; *i.e.*,

$$d(A, B) = \max \left\{ \sup_{a \in A} d(a, B), \sup_{b \in B} d(b, A) \right\}.$$

Let $\tilde{v} : [0, 1] \rightarrow \{-1, +1\}$ be piecewise constant with precisely k discontinuities $\{x_1, x_2, \dots, x_k\} \subset (0, 1)$, and let $v \in U_n$ be its spatial discretization, *i.e.*, $v_i = \tilde{v}(i/n)$. Let r be the largest number such that $(x_j - r, x_j + r) \subset (0, 1)$ for $1 \leq j \leq k$ and $(x_j - r, x_j + r) \cap (x_\ell - r, x_\ell + r) = \emptyset$ for $1 \leq j < \ell \leq k$.

(Throughout this paper v , $\tilde{v}$, r , and k will have the meanings presented here.)

Then our main result is the following:

THEOREM 1.1. *There exists $n_0 = n_0(\rho)$ and $\varepsilon_0 = \varepsilon_0(\rho, k)$, and discretized initial data $u(0)$ within $O(\sqrt{\varepsilon})$ of v that generate solutions $u(t)$ to (1.3) and (1.4) with transition layers moving so slowly that the time necessary for $d(Z(v), Z(u(t)))$ to exceed a fixed value $\rho \leq r$ is greater than*

$$\frac{1}{C_1 \varepsilon} \left(1 + \frac{C_2}{n \varepsilon} \right)^{C_3 n - C_4}$$

for $n \geq n_0$ and $\varepsilon \leq \varepsilon_0$. Here, C_1 , C_2 , C_3 , and C_4 depend on r , k , and ρ , but not on n or ε .

The basic approach that is employed to prove this theorem is based on the variational method developed by Bronsard and Kohn [8] for studying (1.1) and incorporates ideas introduced in [28] that, for the continuous equations, yield exponential, rather than superpolynomial, estimates. (For the discrete equations, these exponential estimates are recovered in the limit as $n \rightarrow \infty$.) We note that the results for the continuous case have been of no direct use to us in the discrete case, since the metastability estimates are subtle enough that they can easily be overwhelmed by discretization error. The relevant estimates seem more difficult to obtain for the lattice equations than for the PDEs because, among other reasons, two parameters must be accounted for rather than just one, and a convenient asymptotic “energy” formula (see, *e.g.*, [34]) is unavailable.

Slow motion has been observed numerically for the Allen-Cahn and Cahn-Hilliard equations in [14], [21], [22] and [33]. Using the Lyapunov function presented in Du and Nicolaides [20] for a full discretization (spatial and temporal), Estep [23] has shown that a temporal discretization of (1.3) inherits the slow motion property for sufficiently fine discretizations. Our results show that transition-layer motion must, in some sense, be slow for (1.3) and (1.4) without requiring a discretization whose fineness depends on ε . In other words, there is a neighborhood of the origin in the first quadrant of the $(\varepsilon, 1/n)$ -plane throughout which the speed of interfaces can be estimated.

It is possible for a time varying solution of (1.1) or (1.2) to become an equilibrium solution of (1.3) or (1.4). This phenomenon is sometimes called *pinning* in the materials science literature, and has been studied for these types of equations by Cahn [10] and others. It is desirable to complement our main result by one which describes what must

happen before interfaces can become pinned. While not, by any means, giving a complete resolution to this problem, the following result yields some information about the spacing of interfaces in a pinned solution to the discrete equations. In the presentation of this result, we will say u_i is a *local maximum (minimum)* if $u_i \geq (\leq) u_j$ for all lattice sites j adjacent to i .

THEOREM 1.2. *Let $u \in U_n$ be a nonconstant equilibrium of (1.3) or of (1.4), and let u_i and u_j be a local minimum and a local maximum, respectively. If $\nu \geq 1/\sqrt{2}$ then*

$$(1.5) \quad |i - j| \geq \left\lfloor \frac{\pi}{\cos^{-1}\left(1 - \frac{1}{2\nu^2}\right)} \right\rfloor - 1.$$

Consequently, the transition layers of a solution u to (1.3) or (1.4), whose speed is bounded by Theorem 1.1, cannot become pinned (at least) until every interval of length

$$\left\lfloor \frac{\pi}{\cos^{-1}\left(1 - \frac{1}{2\nu^2}\right)} \right\rfloor - 1$$

contains no more than two members of $\{0, n\} \cup nZ(u)$.

The paper is organized as follows. In Section 2 an elementary abstract result is presented that shows how to use variational techniques to estimate evolution speeds for a certain class of equations. In Section 3 some basic properties of (1.3) and (1.4) are discussed, in particular the existence of a conserved quantity for (1.4), called *mass*, and a dissipated quantity for (1.3) and (1.4), called *energy*. These properties will ensure that (for the proper choice of space and inner product) these equations fit into the framework of the preceding section. Section 4 contains the construction of initial data very close to v with transition layers with very little excess energy. In Section 5, it is shown that there is a minimum energy cost per interface for any solution with a transition-layer structure, and Theorem 1.1 is then proved. Finally, in Section 6, Theorem 1.2 is proved.

2. Abstract Variational Method. The method that Bronsard and Kohn developed for detecting slowly-evolving solutions is based on a very simple idea: If motion is driven by energy dissipation and if there are solutions that move large distances without losing much energy, then they must move very slowly. In this section this principle is formulated as an abstract result general enough to apply to a large class of both ordinary and partial differential equations. In subsequent sections, we perform the delicate energy estimates necessary in order to apply this abstract result to the particular equations of interest.

Let $(X, \langle \cdot, \cdot \rangle)$ be an inner product space with induced norm $\|\cdot\|$, and let M be a linear manifold in X , *i.e.*, a translate of a linear subspace $\widetilde{M}$. Given a functional $F : M \rightarrow \mathbf{R}$ and a point $x \in M$, we will say that an element $y \in \widetilde{M}$ is the *gradient* of F at x on M (and write $y = \nabla_M F(x)$) if for every differentiable curve $\gamma(t)$ in M satisfying $\gamma(t_0) = x$,

$$\left. \frac{d}{dt} F(\gamma(t)) \right|_{t=t_0} = \langle y, \gamma'(t_0) \rangle.$$

A *gradient flow* for F on M is a differential equation of the form

$$\frac{dx}{dt} = -\kappa \nabla_M F(x)$$

for some positive constant κ .

The following lemma, although quite simple, is really the core of the variational approach to dynamical metastability.

LEMMA 2.1. *Let $x(t)$ be a solution of the gradient flow*

$$\frac{dx}{dt} = -\kappa \nabla_M F(x)$$

on M for $t \geq 0$. Then

$$\|x(t) - x(0)\| \leq \sqrt{\kappa t (F(x(0)) - F(x(t)))}.$$

Proof. Note that

$$\begin{aligned} F(x(0)) - F(x(t)) &= - \int_0^t \frac{d}{d\tau} F(x(\tau)) d\tau = - \int_0^t \langle \nabla_M F(x(\tau)), x'(\tau) \rangle d\tau \\ &= \kappa \int_0^t \|\nabla_M F(x(\tau))\|^2 d\tau \geq \frac{\kappa}{t} \left(\int_0^t \|\nabla_M F(x(\tau))\| d\tau \right)^2 \end{aligned}$$

by Jensen's inequality. Thus,

$$\begin{aligned} \|x(t) - x(0)\| &= \left\| \int_0^t x'(\tau) d\tau \right\| \leq \int_0^t \|x'(\tau)\| d\tau \\ &= \kappa \int_0^t \|\nabla_M F(x(\tau))\| d\tau \leq \sqrt{\kappa t (F(x(0)) - F(x(t)))}. \end{aligned}$$

□

3. Properties of Discrete Equations. Let U_n be as in the Introduction, and define an inner product $\langle \cdot, \cdot \rangle_2$ on U_n by

$$\langle u, v \rangle_2 = \frac{1}{n+1} \sum_{i=0}^n u_i v_i,$$

and set $m = (1, 1, \dots, 1)^T$. Two important real-valued functionals on U_n are the *mass* $\langle m, \cdot \rangle_2$ and the *energy* E , defined by

$$E(u) = \frac{1}{\nu} \sum_{i=0}^n W(u_i) + \frac{\nu}{2} \sum_{i=0}^{n-1} (u_{i+1} - u_i)^2.$$

It will sometimes be necessary to refer to the energy on some set of consecutive integers other than $\{0, 1, \dots, n\}$. In those situations we will write

$$E(u; j, \ell) = \frac{1}{\nu} \sum_{i=j}^{\ell} W(u_i) + \frac{\nu}{2} \sum_{i=j}^{\ell-1} (u_{i+1} - u_i)^2.$$

Let Δ be the linear operator on U_n given by left-multiplication by the tridiagonal matrix

$$\begin{bmatrix} -1 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -1 \end{bmatrix}.$$

(We shall also refer to this matrix itself as Δ .)

If $f : U_n \rightarrow U_n$ is now defined to be the map obtained by applying the real function f componentwise, then (1.3) can be rewritten as a differential equation in U_n :

$$(3.1) \quad \dot{u} = \nu^2 \Delta u - f(u).$$

Similarly, (1.4) can be simplified to the following pair of equations in U_n :

$$(3.2) \quad \begin{aligned} \dot{u} &= -n^2 \Delta \mu(u), \\ \mu(u) &= \nu^2 \Delta u - f(u). \end{aligned}$$

Note that Δ is self-adjoint with respect to $\langle \cdot, \cdot \rangle_2$ and that the null space of Δ is spanned by m . Let $\Delta^\dagger$ be the Moore-Penrose pseudo-inverse of Δ ; *i.e.*, $\Delta^\dagger u$ satisfies $\Delta \Delta^\dagger u = u - \langle m, u \rangle_2 m$ and $\langle m, \Delta^\dagger u \rangle_2 = 0$. Define $\langle \cdot, \cdot \rangle_{-1}$

$$\langle u, v \rangle_{-1} = \langle H u, v \rangle_2,$$

where

$$H = \frac{m m^T}{n+1} - \frac{\Delta^\dagger}{(n+1)^2}.$$

We claim that this is an inner product on U_n . Its bilinearity is clear. Its symmetry follows from the fact that $\Delta^\dagger$ is self-adjoint with respect to $\langle \cdot, \cdot \rangle_2$, which, in turn, follows from the fact that Δ is self-adjoint with respect to $\langle \cdot, \cdot \rangle_2$. It remains only to show that it is positive definite, *i.e.*, that $\langle u, u \rangle_{-1} \geq 0$ with equality only if $u = 0$.

It is well-known that the eigenvalues of $-\Delta$ are

$$\{2(1 - \cos(j\pi/(n+1))) : j = 0, 1, \dots, n\}.$$

Hence, the eigenvalues of $-\Delta^\dagger$ are

$$\{0\} \cup \left\{ [2(1 - \cos(j\pi/(n+1)))]^{-1} : j = 1, \dots, n \right\},$$

and the eigenvalues of H are

$$\{1\} \cup \left\{ [2(n+1)^2(1 - \cos(j\pi/(n+1)))]^{-1} : j = 1, \dots, n \right\}.$$

This proves positive definiteness, so $\langle \cdot, \cdot \rangle_{-1}$ is indeed an inner product.

An application of Taylor's theorem to the eigenvalues of H shows that they lie in the interval $[(2(n+1))^{-2}, 1]$. Thus, if we denote the induced norms corresponding to $\langle \cdot, \cdot \rangle_2$ and $\langle \cdot, \cdot \rangle_{-1}$, $\| \cdot \|_2$ and $\| \cdot \|_{-1}$, respectively, then

$$(3.3) \quad \frac{1}{2(n+1)} \|u\|_2 \leq \|u\|_{-1} \leq \|u\|_2.$$

Now, let $\gamma(t)$ be a curve in U_n . A calculation shows that

$$(3.4) \quad \begin{aligned} \frac{d}{dt} E(\gamma(t)) &= \dot{\gamma}_0(t) [\nu^{-1} f(\gamma_0(t)) - \nu(-\gamma_0(t) + \gamma_1(t))] \\ &\quad + \sum_{i=1}^{n-1} \dot{\gamma}_i(t) [\nu^{-1} f(\gamma_i(t)) - \nu(\gamma_{i-1}(t) - 2\gamma_i(t) + \gamma_{i+1}(t))] \\ &\quad + \dot{\gamma}_n(t) [\nu^{-1} f(\gamma_n(t)) - \nu(\gamma_{n-1}(t) - \gamma_n(t))], \end{aligned}$$

so if we let ℓ_n^2 be the Hilbert space consisting of U_n with inner product $\langle \cdot, \cdot \rangle_2$ then

$$\nabla_{\ell_n^2} E(u) = (n+1)(\nu^{-1}f(u) - \nu\Delta u),$$

and the discrete Allen-Cahn equation can be written

$$(3.5) \quad \dot{u} = -\frac{\nu}{n+1} \nabla_{\ell_n^2} E(u).$$

Next, define h_n^{-1} to be the Hilbert space consisting of U_n with inner product $\langle \cdot, \cdot \rangle_{-1}$, and let h_{n,m_0}^{-1} be the codimension one submanifold of h_n^{-1} consisting of those elements with mass m_0 . From (3.4) we have

$$\frac{d}{dt} E(\gamma(t)) = -\frac{n+1}{\nu} \langle \mu(\gamma(t)), \dot{\gamma}(t) \rangle_2,$$

where μ is as in (3.2). If $\gamma(t)$ is in h_{n,m_0}^{-1} for all t then $\langle m, \dot{\gamma}(t) \rangle_2 = 0$, so

$$\begin{aligned} \frac{d}{dt} E(\gamma(t)) &= -\frac{n+1}{\nu} \langle (-(n+1)mm^T + \Delta^\dagger)\Delta\mu(\gamma(t)), \dot{\gamma}(t) \rangle_2 \\ &= \frac{(n+1)^3}{\nu} \langle H\Delta\mu(\gamma(t)), \dot{\gamma}(t) \rangle_2 = \frac{(n+1)^3}{\nu} \langle \Delta\mu(\gamma(t)), \dot{\gamma}(t) \rangle_{-1}. \end{aligned}$$

Thus,

$$\nabla_{h_{n,m_0}^{-1}} E(u) = \frac{(n+1)^3}{\nu} \Delta\mu(u),$$

and the discrete Cahn-Hilliard equation can be written

$$(3.6) \quad \dot{u} = -\frac{n^2\nu}{(n+1)^3} \nabla_{h_{n,m_0}^{-1}} E(u).$$

4. Efficient Initial Data. Since both (3.1) and (3.2) are gradient flows for E , Lemma 2.1 will eventually provide an estimate on the rate at which solutions evolve, if the energy decay can be estimated. In this section, initial data for the discrete equations are generated that are close to the discretized step function v and that have efficient transition layers. Before stating the result, we introduce the quantity

$$E_\nu \stackrel{\text{def}}{=} \inf \left\{ E(z; -\infty, +\infty) : \lim_{i \rightarrow \pm\infty} z_i \text{sgni} = 1 \right\}.$$

LEMMA 4.1. *There exists $u(0) \in U_n$ and a constant B such that*

$$(4.1) \quad E(u(0)) \leq kE_\nu$$

and

$$(4.2) \quad \|u(0) - v\|_\sigma^2 \leq Bk\varepsilon, \quad \sigma = -1, 2.$$

Furthermore,

$$(4.3) \quad E_\nu \leq \min(2\nu, 2\sqrt{2}/3).$$

Proof. We construct the transition layers of $u(0)$ out of pieces of a profile realizing the infimum in the definition of E_ν . First, we show that such a minimizer exists. Let $z^{(1)}, z^{(2)}, z^{(3)}, \dots$ be a minimizing sequence; i.e., $E(z^{(j)}; -\infty, +\infty) \rightarrow E_\nu$ as $j \rightarrow \infty$. Note that $E(\zeta; -\infty, +\infty) \leq E(z^{(j)}; -\infty, +\infty)$, where $\zeta = \min(1, \max(-1, z^{(j)}))$. Also, note that all strictly decreasing segments of ζ have finite length and if ξ is obtained from ζ by reversing each of its maximal decreasing segments then $E(\xi; -\infty, +\infty) \leq E(\zeta; -\infty, +\infty)$. Thus, without loss of generality we can assume that $z_i^{(j)}$ is contained in $[-1, 1]$ and is monotone increasing in i . Because E is translationally invariant, we may also assume that $z_{-1}^{(j)} \leq 0$ and $z_0^{(j)} \geq 0$. For fixed i , $z_i^{(j)}$ is a bounded sequence and, therefore, has a convergent subsequence. By a Cantor diagonalization process we can obtain a subsequence $z^{(j_\ell)}$ of $z^{(j)}$ that converges at every i . Call the pointwise limit z .

Note that z_i is contained in $[-1, 1]$ and is a nondecreasing function of i , and that $z_{-1} \leq 0$ and $z_0 \geq 0$. We claim that z has the correct limiting behavior at $\pm\infty$ so that z is an admissible function for the minimization problem. To see why this must be so, observe that the monotonicity of $z^{(j)}$ implies that

$$\frac{|i|}{\nu} W(z_i^{(j)}) \leq \max_j E(z^{(j)}; -\infty, +\infty),$$

so $z_i^{(j)} \text{sgn} i \rightarrow 1$ uniformly in j as $i \rightarrow \pm\infty$. Hence, the pointwise limit z must have the same convergence property. Finally, note that

$$\begin{aligned} E(z; -\infty, +\infty) &= \lim_{N \rightarrow \infty} E(z; -N, +N) = \lim_{N \rightarrow \infty} \lim_{\ell \rightarrow \infty} E(z^{(j_\ell)}; -N, +N) \\ &\leq \lim_{N \rightarrow \infty} \lim_{\ell \rightarrow \infty} E(z^{(j_\ell)}; -\infty, +\infty) = E_\nu. \end{aligned}$$

This minimizer is not necessarily unique (even up to translation). Pick one such minimizer and call it z^ν .

Let $d_i = \min\{|i - j| : v_j \neq v_i\}$. Then the initial data $u(0)$ will be given by

$$u_i(0) = \begin{cases} z_{d_i-1}^\nu & \text{if } v_i = +1 \\ z_{-d_i}^\nu & \text{if } v_i = -1 \end{cases}$$

Clearly, (4.1) holds. The distance from $u(0)$ to v can be estimated as follows:

$$(4.4) \quad \|u(0) - v\|_2^2 \leq \frac{k}{n+1} \sum_{i=-\infty}^{+\infty} (1 - |z_i^\nu|)^2 \leq \frac{4k}{n+1} \sum_{i=-\infty}^{+\infty} W(z_i^\nu).$$

Now pick $j \in \{0, 1\}$ such that

$$\sum_{i=-\infty}^{+\infty} W(z_{2i+j}^\nu) \leq \frac{1}{2} \sum_{i=-\infty}^{+\infty} W(z_i^\nu),$$

and let $\zeta_i = z_{2i+j}^\nu$. Then by the optimality of z^ν ,

$$\begin{aligned} E_\nu &\leq \sum_{i=-\infty}^{+\infty} \left[\frac{1}{\nu} W(\zeta_i) + \frac{\nu}{2} (\zeta_{i+1} - \zeta_i)^2 \right] \\ &\leq \frac{1}{2\nu} \sum_{i=-\infty}^{+\infty} W(z_i^\nu) + \nu \sum_{i=-\infty}^{+\infty} (z_{i+1}^\nu - z_i^\nu)^2 = 2E_\nu - \frac{3}{2\nu} \sum_{i=-\infty}^{+\infty} W(z_i^\nu). \end{aligned}$$

Hence,

$$\sum_{i=-\infty}^{+\infty} W(z_i^\nu) \leq \frac{2\nu}{3} E_\nu,$$

and

$$(4.5) \quad \|u(0) - v\|_2^2 \leq \frac{8k\nu}{3(n+1)} E_\nu.$$

Now, evaluation of $E(\cdot; -\infty, +\infty)$ at the admissible function $z_i = \tanh(i/(\nu\sqrt{2}))$ shows that $\limsup_{\nu \rightarrow \infty} E_\nu \leq 2\sqrt{2}/3$. Furthermore, by evaluating the energy of the admissible function $z_i = z_{2i+j}^{2\nu}$, where $j \in \{0, 1\}$ is such that

$$\sum_{i=-\infty}^{+\infty} W(z_{2i+j}^{2\nu}) \leq \frac{1}{2} \sum_{i=-\infty}^{+\infty} W(z_i^{2\nu}),$$

it can be seen that $E_\nu \leq E_{2\nu}$ for any ν . Thus, $E_\nu \leq 2\sqrt{2}/3$ for all ν . Calculation of $E(z; -\infty, +\infty)$ for $z_i = \text{sgn}(i + 1/2)$ completes the verification of (4.3). Substituting (4.3) into (4.5) yields (4.2), for $\sigma = 2$. From (3.3), we also get (4.2) for $\sigma = -1$. $\square$

5. Minimum Energy of Transition-Layer Solutions. This section begins with three technical lemmas. The first lemma relates norm estimates to pointwise estimates.

LEMMA 5.1. *Suppose that $z \in U_n$ and that S_q is a set of q consecutive sites in the lattice. Then:*

1. *If $\|z\|_2 \leq \delta$ then $z_i \leq \delta \sqrt{\frac{n+1}{q}}$ for some $i \in S_q$.*
 2. *If $\|z\|_{-1} \leq \delta$ then $z_i \leq \delta \sqrt{\frac{13(n+1)^3}{q^3}}$ for some $i \in S_q$.*
- Proof.* Suppose $\|z\|_2 \leq \delta$. If $z_i > Z > 0$ for all $i \in S_q$, then

$$\delta^2 \geq \|z\|_2^2 = \frac{1}{n+1} \sum_{i=0}^n z_i^2 > \frac{qZ^2}{n+1},$$

so $Z < \delta \sqrt{\frac{n+1}{q}}$. This proves part 1.

Suppose now that $\|z\|_{-1} \leq \delta$ and that $z_i > Z > 0$ for all $i \in S_q$. Observe that $\Delta^\dagger = -(D^{-1}P)^T D^{-1}P$, where

$$P = I - \frac{mm^T}{n+1},$$

and D^{-1} is the matrix with ones on and below the main diagonal and zeros above it. Then

$$\|z\|_{-1}^2 = \langle Hz, z \rangle_2 = \frac{(m^T z)^2}{(n+1)^2} + \frac{1}{(n+1)^2} \langle D^{-1}Pz, D^{-1}Pz \rangle_2.$$

Setting $\beta = (m^T z)/(n+1)$ gives

$$\|z\|_{-1}^2 = \beta^2 + \frac{1}{(n+1)^3} \sum_{i=0}^n \left(\sum_{j=0}^i (z_j - \beta) \right)^2 \geq \min_{\hat{\alpha}, \hat{\beta}} F(\hat{\alpha}, \hat{\beta}),$$

where

$$F(\hat{\alpha}, \hat{\beta}) \stackrel{\text{def}}{=} \hat{\beta}^2 + \frac{1}{(n+1)^3} \sum_{i=0}^q (\hat{\alpha} + i(Z - \hat{\beta}))^2.$$

It is easy to verify that

$$\min_{\hat{\alpha}, \hat{\beta}} F(\hat{\alpha}, \hat{\beta}) = \frac{q^3 + 3q^2 + 2q}{12(n+1)^3 + q^3 + 3q^2 + 2q} Z^2,$$

so

$$Z \leq \delta \sqrt{\frac{12(n+1)^3}{q^3 + 3q^2 + 2q} + 1} \leq \delta \sqrt{\frac{13(n+1)^3}{q^3}}.$$

This proves part 2. $\square$

The second lemma estimates the decay rate of an energy minimizer at one end of a finite lattice subject to a boundary condition at the other end.

LEMMA 5.2. *Given $z_0 \in [0, 1)$, let z_i , ($i = 1, 2, \dots, p$), minimize $E(z - 1; 0, p)$. Then*

$$(5.1) \quad z_p \leq \frac{2z_0}{\left[1 + \nu^{-1} \sqrt{(1 - z_0)(2 - z_0)}\right]^p}.$$

Proof. Calculus implies that z must satisfy

$$z_i = 2z_{i+1} - z_{i+2} + \frac{1}{\nu^2} f(z_{i+1} - 1)$$

for $i = 0, 1, \dots, p - 2$, and

$$z_{p-1} = z_p + \frac{1}{\nu^2} f(z_p - 1).$$

Also, z_i must be in $[0, z_0]$ for each i . Thus, f can be bounded from below to give the estimates

$$z_i \geq \alpha z_{i+1} - z_{i+2}$$

for $i = 0, 1, \dots, p - 2$, and

$$z_{p-1} \geq (\alpha - 1)z_p,$$

where

$$\alpha = 2 + \nu^{-2}(1 - z_0)(2 - z_0).$$

For $i = 0, 1, \dots, p + 1$, define

$$a_i = \frac{R^{1+i} - R^{1-i}}{R^2 - 1}$$

where

$$R = \frac{\alpha}{2} + \sqrt{\left(\frac{\alpha}{2}\right)^2 - 1}.$$

It is easy to see that a_i satisfies the recurrence relation $a_i = \alpha a_{i-1} - a_{i-2}$ with initial conditions $a_0 = 0$, $a_1 = 1$. Also, note that $R > 1$, so $a_i \geq 0$.

By induction on i it can be shown that

$$(5.2) \quad z_0 \geq a_{i+1}z_i - a_i z_{i+1}$$

for $j = 0, 1, \dots, p-1$. In particular, (5.2) holds for $i = p-1$, so

$$\begin{aligned} z_0 &\geq a_p z_{p-1} - a_{p-1} z_p \geq [a_p(\alpha - 1) - a_{p-1}] z_p = (a_{p+1} - a_p) z_p \\ &= \frac{(R^{1+p} + R^{-p}) z_p}{R+1} \geq \frac{R^p z_p}{2} \geq \frac{\left[1 + \nu^{-1} \sqrt{(1-z_0)(2-z_0)}\right]^p z_p}{2}. \end{aligned}$$

This implies (5.1). $\square$

The third lemma gives an upper bound for the minimal energy on a semi-infinite lattice.

LEMMA 5.3. *Given $z_0 \in [0, 1)$, there exists a sequence $z_1, z_2, \dots$ converging to 0 such that*

$$E(z-1; 0, \infty) - \nu^{-1} W(z_0 - 1) \leq \nu z_0^2 / (1 + \nu\sqrt{2}).$$

Proof. Set $z_i = z_0 R^{-i}$ where $R = 1 + \nu^{-1}\sqrt{2}$. A computation shows that

$$E(z-1; 0, \infty) - \nu^{-1} W(z_0 - 1) \leq z_0^2 \left[\frac{(R-1)\nu}{2(R+1)} + \frac{1}{\nu(R-1)(R+1)} \right] = \frac{\nu z_0^2}{1 + \nu\sqrt{2}}.$$

$\square$

These three lemmas can be combined to give a lower bound on $E(u)$ if u is close to v in ℓ_n^2 or in h_n^{-1} .

LEMMA 5.4. *Suppose*

$$(5.3) \quad \|u - v\|_\sigma \leq \delta$$

where $\sigma = -1$ or 2 , (and v is the discretized step function). Then there are positive constants C_2, C_3, C_4 , and C_5 (depending on k, r , and δ , but not on ε or n) such that

$$(5.4) \quad E(u) \geq kE_\nu - C_5 \left[1 + \frac{C_2}{n\varepsilon} \right]^{-C_3 n + C_4}$$

for $\delta \leq \frac{nr-1}{(n+1)\sqrt{r}}$ when $\sigma = 2$, and for $\delta^4 \leq \frac{(nr-1)^9}{169r^3(n+1)^9}$ when $\sigma = -1$.

Proof. Suppose $\|u - v\|_2 \leq \delta$ and that $v_j = -1$ and $v_{j+1} = +1$ for some j . Set $q = \lceil \delta(n+1)\sqrt{r} \rceil$ and apply Lemma 5.1 with $z = u - v$ to get $u_\ell \leq -1 + z^*$ for some $\ell \in S_q \equiv \{j - q + 1, j - q + 2, \dots, j\}$, where $z^* = \delta\sqrt{(n+1)/q}$. Similarly, $u_\ell \geq 1 - z^*$ for some $\ell \in \{j + 1, j + 2, \dots, j + q\}$. Set $p = \lceil nr \rceil - \lceil \delta(n+1)\sqrt{r} \rceil - 1$. By Lemma 5.2,

$$(5.5) \quad E(u; j - p - q + 1, j + q + p) \geq E(\phi; j - p - q + 1, j + q + p)$$

for some ϕ satisfying

$$\phi_{j-p-q+1} \leq -1 + \frac{2z^*}{\left[1 + \nu^{-1} \sqrt{(1-z^*)(2-z^*)}\right]^p}$$

and

$$\phi_{j+q+p} \geq 1 - \frac{2z^*}{\left[1 + \nu^{-1}\sqrt{(1-z^*)(2-z^*)}\right]^p}.$$

(The function ϕ is obtained by replacing the tails of u by the optimally decaying tails discussed in Lemma 5.2.) Thus, by Lemma 5.3,

$$E(\phi; j-p-q+1, j+q+p) \geq E_\nu - \frac{8\nu(z^*)^2}{(1+\nu\sqrt{2}) \left[1 + \nu^{-1}\sqrt{(1-z^*)(2-z^*)}\right]^{2p}},$$

since otherwise ϕ could be extended to all of $\mathbf{Z}$ so as to be an admissible function for the minimization problem defining E_ν yet have energy less than E_ν , which is a contradiction. By (5.5),

$$(5.6) \quad E(u; j-p-q+1, j+q+p) \geq E_\nu - \frac{8\nu(z^*)^2}{(1+\nu\sqrt{2}) \left[1 + \nu^{-1}\sqrt{(1-z^*)(2-z^*)}\right]^{2p}}.$$

Clearly (5.6) also holds when $v_j = +1$ and $v_{j+1} = -1$.

If δ is as in the theorem statement, then as j ranges over all jumps in v , (5.6) estimates the energy of u over disjoint sublattices of $\{0, 1, \dots, n\}$. We can, therefore, sum (5.6) over all k jumps and simplify to get (5.4) for $\sigma = 2$.

The proof for $\sigma = -1$ is similar. In this case, we can set $q = \lceil (169\delta^4 r^3)^{1/9}(n+1) \rceil$, $z^* = \delta\sqrt{13((n+1)/q)^3}$, and $p = \lceil nr \rceil - \lceil (169\delta^4 r^3)^{1/9}(n+1) \rceil - 1$ to obtain (5.4). $\square$

There are two more lemmas before the proof of the main result. The first of these gives a lower bound on the energy of a profile that is near ± 1 at some sites and takes on values of the opposite sign at other sites. The second uses the first to establish a relationship between the distance between v and u in ℓ_n^2 or h_n^{-1} and the Hausdorff distance between their zero sets, if it is assumed that u has efficient transition layers.

LEMMA 5.5. *Suppose $|z_0| \geq 1/\sqrt{3}$ and $z_0 z_j \leq 0$ for some $j \in \mathbf{N}$. Then*

$$(5.7) \quad E(z; 0, j) - \nu^{-1}W(z_0) \geq \min(2\nu/3, (\sqrt{6})/9).$$

Furthermore, if $|z_j| \geq 1/\sqrt{3}$ then

$$(5.8) \quad E(z; 0, j) - \nu^{-1}(W(z_0) + W(z_j)) \geq \min(2\nu/3, (\sqrt{6})/9).$$

Proof. Without loss of generality, assume $z_0 < 0$. Set $\widehat{W}(u)$ to be $1/9$ for $|u| < 1/\sqrt{3}$ and 0 elsewhere. Note that, since $\widehat{W}(u) \leq W(u)$, to prove (5.7) and (5.8) it suffices to show that

$$(5.9) \quad \widehat{E} \geq \min(2\nu/3, (\sqrt{6})/9),$$

where

$$\widehat{E} = \widehat{E}(z_0, z_1, \dots, z_j; j) = \sum_{i=1}^j \left[\frac{1}{\nu} \widehat{W}(z_i) + \frac{\nu}{2} (z_i - z_{i-1})^2 \right]$$

It is not hard to see that if j and $(z_0, z_1, \dots, z_j)$ minimize $\hat{E}$ then either $z_i = (2i - 1)/\sqrt{3}$ and $j = 1$, or $z_i = (i/j - 1)/\sqrt{3}$ and $j \geq 1$. In the first case, $\hat{E} = 2\nu/3$, and in the second case

$$\hat{E} = \min_{j \in \mathbf{N}} \left[\frac{j}{9\nu} + \frac{\nu}{6j} \right] \geq \min_{x \in \mathbf{R}^+} \left[\frac{x}{9} + \frac{1}{6x} \right] = \frac{\sqrt{6}}{9}.$$

Thus, (5.9) holds. $\square$

LEMMA 5.6. *If $\|u - v\|_2 \leq \delta$ and $E(u) \leq kE_\nu$ then*

$$(5.10) \quad d(Z(u), Z(v)) \leq \frac{\lfloor 6\delta^2 k(n+1) \rfloor + 1/2}{n}.$$

If $\|u - v\|_{-1} \leq \delta$ and $E(u) \leq kE_\nu$ then

$$(5.11) \quad d(Z(u), Z(v)) \leq \frac{\lfloor (78\delta^2 k)^{1/3}(n+1) \rfloor + 1/2}{n}.$$

Proof. Suppose $\|u - v\|_2 \leq \delta$ and $E(u) \leq kE_\nu$, and set $q = \lfloor 6\delta^2 k(n+1) \rfloor + 1$, and $z^* = \delta\sqrt{(n+1)/q} \leq 1 - 1/\sqrt{3}$. For each discontinuity in $\tilde{v}$, Lemma 5.1 shows that u takes on a value less than $-1 + z^*$ within the first q lattice sites on one side and a value greater than $1 - z^*$ within the first q lattice sites on the opposite side. By Lemma 5.3, the energy of u between these two sites is no less than $E_\nu - 2\nu(z^*)^2/(1 + \nu\sqrt{2})$. Considering all k discontinuities of $\tilde{v}$, we see that an energy of at least

$$(5.12) \quad kE_\nu - 2k\nu(z^*)^2/(1 + \nu\sqrt{2})$$

is expended within q sites of the discontinuities. If there were a zero of u more than q lattice sites away from a discontinuity in $\tilde{v}$ then by Lemma 5.5 the extra energy needed to achieve this would be at least $\min(2\nu/3, (\sqrt{6})/9)$. Adding this to (5.12) would give a contradiction, in light of (4.3). Hence,

$$(5.13) \quad \max_{x \in Z(u)} d(x, Z(v)) \leq \frac{q - 1/2}{n}.$$

Also, the Intermediate Value Theorem implies that

$$(5.14) \quad \max_{x \in Z(v)} d(x, Z(u)) \leq \frac{q - 1/2}{n}.$$

Combining (5.14) and (5.13) yields (5.10).

If $\|u - v\|_{-1} \leq \delta$, then setting $q = \lfloor (78\delta^2 k)^{1/3}(n+1) \rfloor + 1$ and reasoning as above, we obtain (5.11). $\square$

Proof of Theorem 1.1. We give the proof for (1.3); the result for (1.4) can be handled similarly. Pick $n_0 = n_0(\rho)$ large enough that

$$0 < \frac{2\rho n_0 - 1}{12(n_0 + 1)} \leq \frac{(n_0\rho - 1)^2}{\rho(n_0 + 1)^2}$$

and set $\delta^2 = (2\rho n_0 - 1)/(12(n_0 + 1)k)$. Pick $\varepsilon_0 = \varepsilon_0(\rho, k)$ small enough that $4Bk\varepsilon_0 \leq \delta^2$. Assume $n \geq n_0$ and $\varepsilon \leq \varepsilon_0$, and apply Lemma 4.1 to get initial data $u(0) \in U_n$ satisfying $E(u(0)) \leq kE_\nu$ and $\|u(0) - v\|_2^2 \leq Bk\varepsilon$, and let $u(t)$ be the corresponding solution of

(3.1). Suppose $d(Z(v), Z(u(t))) \geq \rho$. Then since $E(u(t)) \leq E(u(0))$, the estimate (5.10) in Lemma 5.6 implies that $\|u(t) - v\|_2 \geq \delta$. Also by the choice of n_0 and ε_0 , $\|u(0) - v\|_2 \leq \delta/2$, so there is a first $T \in (0, t]$ such that $\|u(T) - v\|_2 = \delta$.

By our choice of n_0 , we are able to apply Lemma 5.4 to obtain

$$E(u(T)) \geq kE_\nu - C_5 \left[1 + \frac{C_2}{n\varepsilon} \right]^{-C_3n+C_4}.$$

Thus,

$$(5.15) \quad \|u(T) - u(0)\|_2 \geq \|u(T) - v\|_2 - \|u(0) - v\|_2 \geq \delta/2,$$

and

$$(5.16) \quad E(u(0)) - E(u(T)) \leq \frac{C_5}{\left[1 + \frac{C_2}{n\varepsilon} \right]^{C_3n-C_4}}.$$

Applying Lemma 2.1 to (3.5) and using (5.15) and (5.16) yields

$$T \geq \frac{1}{C_1\varepsilon} \left(1 + \frac{C_2}{n\varepsilon} \right)^{C_3n-C_4}.$$

□

6. Properties of Equilibria.

Proof of Theorem 1.2. Because it is an equilibrium, u must satisfy

$$(6.1) \quad \nu^2 \Delta u = f(u) + \alpha m$$

for some constant α . Extend u to $\ell = n+1, \dots, 2n+1$ by the formula $u_\ell = u_{2n+1-\ell}$, and then extend it to be a $(2n+2)$ -periodic function on all of $\mathbf{Z}$. Define $w_\ell = u_\ell - u_{\ell-1}$, and note that (6.1) implies that

$$(6.2) \quad \nu^2(w_{\ell-1} - 2w_\ell + w_{\ell+1}) = f(u_\ell) - f(u_{\ell-1}),$$

for all $\ell \in \mathbf{Z}$. Since $f' \geq -1$, the Mean Value Theorem applied to (6.2) yields

$$(6.3) \quad w_{\ell+1} \geq \left(2 - \frac{1}{\nu^2} \right) w_\ell - w_{\ell-1}$$

if $w_\ell \geq 0$.

Now suppose u_i is a local minimum, so $w_i \leq 0$ and $w_{i+1} \geq 0$. We shall prove that, in fact, $w_{i+j} \geq 0$ for $j = 1, 2, \dots, p$, where

$$p = \left\lfloor \frac{\pi}{\cos^{-1}\left(1 - \frac{1}{2\nu^2}\right)} \right\rfloor.$$

To do this we will use the auxiliary sequence $a_\ell = \frac{\sin \ell\theta}{\sin \theta}$, where $\theta = \cos^{-1}(1 - 1/(2\nu^2))$. Since $\nu \geq 1/\sqrt{2}$, $\theta \in (0, \pi/2]$, so this sequence is well-defined. Note that $a_0 = 0$, $a_1 = 1$, $a_2 = 2 - 1/\nu^2$, and $a_{\ell+1} = a_2 a_\ell - a_{\ell-1}$. Note also that $a_\ell \geq 0$ for $\ell = 0, 1, \dots, p$.

Now, let P_j be the proposition that $w_{i+1} \geq 0, w_{i+2} \geq 0, \dots, w_{i+j} \geq 0$. We will prove P_j for $j = 1, \dots, p$ by induction on j . Also, let $Q_{j,\ell}$ be the proposition that $w_{i+j+1} \geq$

$a_\ell w_{i+j+2-\ell} - a_{\ell-1} w_{i+j+1-\ell}$. For fixed $j < p$, we will prove $Q_{j,\ell}$ for $\ell = 1, \dots, j+1$ by induction on ℓ .

P_1 is the statement $w_{i+1} \geq 0$, which is true by assumption. Suppose P_j is true, for some $j < p$. Fix j , and note that $Q_{j,1}$ is the statement $w_{i+j+1} \geq w_{i+j+1}$, which is, of course, true. Suppose $Q_{j,\ell}$ holds for some $\ell \leq j$. Since $i+1 \leq i+j+1-\ell \leq i+j$, P_j implies that $w_{i+j+1-\ell} \geq 0$. Also, $a_\ell \geq 0$, since $\ell \leq j < p$. Thus, (6.3) and $Q_{j,\ell}$ imply that

$$\begin{aligned} w_{i+j+1} &\geq a_\ell w_{i+j+2-\ell} - a_{\ell-1} w_{i+j+1-\ell} \geq a_\ell [(2 - \nu^{-2}) w_{i+j+1-\ell} - w_{i+j-\ell}] - a_{\ell-1} w_{i+j+1-\ell} \\ &= (a_\ell a_2 - a_{\ell-1}) w_{i+j+1-\ell} - a_\ell w_{i+j-\ell} = a_{\ell+1} w_{i+j+2-(\ell+1)} - a_{(\ell+1)-1} w_{i+j+1-(\ell+1)}, \end{aligned}$$

so $Q_{j,\ell+1}$ holds. By induction, $Q_{j,\ell}$ holds for $\ell = 1, \dots, j+1$. In particular, we have $Q_{j,j+1}$:

$$w_{i+j+1} \geq a_{j+1} w_{i+1} - a_j w_i \geq 0,$$

so P_{j+1} holds. By induction, P_j holds for $j = 1, \dots, p$. In particular, we have P_p :

$$w_{i+1} \geq 0, \dots, w_{i+p} \geq 0,$$

verifying the earlier claim. This implies that if u_j is a local maximum for (the extended) u and $j > i$ then $j \geq i + p - 1$, so $|i - j| \geq p - 1$. A similar result holds if $j < i$. Clearly, the same estimate holds for the original $u \in U_n$, so the proof of (1.5) is complete. The second half of Theorem 1.2 is an immediate consequence. $\square$

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