Journal of Statistical Physics, Vol. 80, Nos. 1/2, 1995

The Classical Statistical Mechanics of Frenkel–Kontorova Models

R. S. MacKay[1]

Received September 7, 1994; final January 19, 1995

The scaling properties of the free energy, specific heat, and mean spacing are calculated for classical Frenkel–Kontorova models at low temperature, in three regimes: near the integrable limit, the anti-integrable limit, and the sliding–pinned transition ("transition by breaking of analyticity"). In particular, the renormalization scheme given in previous work for ground states of Frenkel–Kontorova models is extended to nonzero-temperature Gibbs states, and the hierarchical melting phenomenon of Vallet, Schilling, and Aubry is put on a rigorous footing.

KEY WORDS: Renormalization; scaling; specific heat; anti-integrable limit; sliding–pinned transition.

1. INTRODUCTION

The Frenkel–Kontorova model and its generalizations are models for one-dimensional incommensurate structures.[5] They consist of a one-dimensional array of classical variables $(x_n)_{n\in\mathbb{Z}}$ with momenta p_n and Hamiltonian

$$H=\sum_{n\in Z}\frac{p_n^2}{2m}+h(x_n, x_{n+1}) \tag{1.1}$$

Here, $h\colon \mathbb{R}^2\to\mathbb{R}$ is a function (called the *generating function*) with the following two properties:

$$h(x, x')=h(x+1, x'+1) \tag{1.2}$$

$$h_{12}(x, x')<0 \tag{1.3}$$

[1] Nonlinear Systems Laboratory, Mathematics Institute, University of Warwick, Coventry CV4 7AL, U.K., and Centre de Dynamique des Systèmes Complexes/Laboratoire de Topologie URA CNRS 755, Département de Mathématiques, Université de Bourgogne, BP 138, 21004 Dijon, France.

0022-4715/95/0700-0045$07.50/0

where subscript $i \in \{1, 2\}$ denotes the partial derivative with respect to the ith argument.

The Frenkel–Kontorova model is the special case

$$h(x, x') = \frac{1}{2} t(x' - x - a)^2 + \frac{\lambda}{4\pi^2} \cos 2\pi x \tag{1.4}$$

with parameters t, a, and λ. By choosing appropriate scales in time and energy, it is clear that the dependence on t and λ is only through their ratio

$$k = \lambda / t \tag{1.4a}$$

Also, m in (1.1) can be chosen to be 1.

It will sometimes be convenient to write the Frenkel–Kontorova model in an alternative form. By expanding the square in (1.4), we can write (1.4) as

$$h(x, x') = \frac{1}{2} t(x' - x)^2 - at(x' - x) + \frac{1}{2} ta^2 + \frac{\lambda}{4\pi^2} \cos 2\pi x \tag{1.5}$$

As the term $\frac{1}{2} ta^2$ serves only to shift the origin of energy, we may remove it (except when variations with respect to a or t are required). Denoting

$$P = -at \tag{1.6}$$

we can write Frenkel-Kontorova model in the form

$$h(x, x') = h_{t,\lambda}(x, x') + P(x' - x) \tag{1.7}$$

with

$$h_{t,\lambda}(x, x') = \frac{1}{2} t(x' - x)^2 + \frac{\lambda}{4\pi^2} \cos 2\pi x \tag{1.8}$$

I refer to P as the *pressure* because it is conjugate to the volume (length of the chain in this case). Other authors refer to it (after a sign change) as the *chemical potential*. It will be useful to add a term $P(x' - x)$ to every model (except at the anti-integrable limit, when P should be scaled by t). So we consider models with two parameters, one like k in (1.4a) and one like P or a.

The goal of this paper is to understand the behavior of Frenkel–Kontorova models at low temperatures. Since they are one-dimensional systems with short-range interactions, there is always a unique Gibbs state

for temperature $T>0$ (so no phase transitions at $T>0$), but in a sense there is a phase transition at $T=0$ whose nature depends on which side of a certain fractal "curve" in the (k, P) plane the system is located.

There are two important limits in the (k, P) plane. Models for which h depends only on $(x'-x)$ are called *integrable*, e.g., $\lambda=0$ in (1.4). Models for which h depends only on x are called *anti-integrable*, e.g., $t=0$ in (1.4) [to include this case, condition (1.3) must be weakened to $h_{12}(x, x')\leqslant 0$]. A renormalization operator can be defined for which both these limits are attracting.[13] The basin of attraction of the integrable limit is called the *subcritical* regime, and that for the anti-integrable limit is called the *supercritical* regime. In between is a *critical set* which separates the two basins. Near this critical set particularly interesting scaling relations will be exhibited.

Aspects of this problem have already been studied. Aubry classified the minimum-energy states,[5] proving in particular that they have a well-defined mean spacing[2]

$$\rho=\langle x_{n+1}-x_n\rangle \tag{1.9}$$

and proved basic properties of the $T=0$ phase diagram, such as continuity of ρ.[3] Sinai[20] and Lazutkin and Terman [12] proved that the Gibbs states for $T>0$ converge to a measure supported by the minimum-energy states of a definite mean spacing. The scaling of the $T=0$ phase diagram about the critical set is described in ref. 13. Vallet, *et al.*[19, 23, 24] described aspects of the phase diagram in the supercritical regime, in particular, a hierarchy of Schottky anomalies, and gave an approximate renormalization scheme to explain this.

Here, a complete picture is given for scaling properties for small T, at the integrable and anti-integrable limits, in the subcritical and supercritical regimes, at criticality and near criticality. Remarkable scaling laws are found for the free energy, specific heat capacity, and mean spacing. A rigorous renormalization scheme is presented and hierarchical melting deduced.

We begin in Section 2 by recalling some basics of statistical mechanics. In Sections 3 and 4, respectively, the integrable and anti-integrable limits and their neighborhoods are discussed. The main novelty of the paper lies in Section 5, where a renormalization approach is developed which sheds much light on the transition regime. The paper concludes in Section 6 with a short discussion.

[2] Warning: In physics, the symbol ρ would normally represent a density, e.g., the reciprocal of the mean spacing; my usage here comes from dynamical systems, where the mean spacing is interpreted as a "rotation number."

2. BASICS

The procedure of statistical mechanics (e.g., ref. 6) is to compute

$$z := \lim_{N \to \infty} N^{-1} \log Z_N \tag{2.1}$$

where Z_N is the *partition function*

$$Z_N := \int \exp[-\beta H_N(x, p)]\, d\mu(x, p) \tag{2.2}$$

where $\beta := 1/T$ (in energy units), H_N is the Hamiltonian for a finite part of the system given by restricting the sum in (1.1) to $n = 0$ to $N-1$, with some choice of boundary conditions, and the integral is taken over all phase space for the finite system, with Liouville measure μ. Then the energy per site is given by

$$e = -\partial z/\partial \beta \tag{2.3}$$

and the specific heat at constant pressure P by

$$C_P = \partial e/\partial T = \beta^2\, \partial e/\partial \beta \tag{2.4}$$

Similarly, the mean spacing ρ is given by

$$\rho = -\beta^{-1}\, \partial z/\partial P \tag{2.5}$$

The specific heat at constant ρ (which we shall denote by a subscript V for volume) is obtained by

$$C_V = C_P - (\partial e/\partial P)/(\partial \rho/\partial P) \tag{2.5a}$$

For the Frenkel–Kontorova models (1.1), we take the finite truncations to consist of a chain of N atoms with free ends. Configurations $(x_0, ..., x_N)$ and $(x_0 + 1, ..., x_N + 1)$ are regarded as equivalent when the integral (2.2) is carried out.

The integral (2.2) decomposes into a product $Z_{N,X} Z_{N,P}$ of integrals over configuration and momentum space, leading to a decomposition

$$z = z_X + z_P \tag{2.5b}$$

The momentum-space integral yields

$$z_P = \tfrac{1}{2} \log(2\pi m/\beta) \tag{2.6}$$

The configuration-space integral

$$Z_{N,x} = \int \prod_{n=0}^{N-1} \exp[-\beta h(x_n, x_{n+1})] \prod dx_n \tag{2.7}$$

can be treated in several ways.

A standard way is to recognize (2.7) as approximately Tr L^N, where L is the *transfer operator*

$$(L\phi)(x') = \int dx \exp[-\beta h(x, x')]\, \phi(x) \tag{2.8}$$

Since L is a positive operator, it has a unique eigenvalue μ of maximum modulus and it is real, positive, and simple. Hence

$$z_x = \log \mu \tag{2.9}$$

The largest eigenvalue has positive eigenvector ϕ. Thus no generality is lost in writing it as

$$\phi(x) = \exp[-\beta S(x)] \tag{2.10}$$

and the eigenvalue equation becomes

$$\mu \exp[-\beta S(x')] = \int dx \exp\{-\beta[h(x, x') + S(x)]\} \tag{2.10a}$$

For β large, the integral can be approximated by the saddle-point method:

$$\mu \exp[-\beta S(x')] \simeq \sum \exp\{-\beta[h(x_m, x') + S(x_m)]\} \left[\frac{2\pi}{\beta U''(x_m)}\right]^{1/2} \tag{2.11}$$

where the sum is over local minima $x_m(x')$ of

$$U(x) = h(x, x') + S(x) \tag{2.12}$$

all assumed to be nondegenerate with $U'''(x) \ll \beta^{1/2} U''(x_m)^{3/2}$. If there is a unique global minimum $x_m(x')$ and all other local minima are considerably higher, then for large β the sum (2.11) reduces to one term,

$$\mu \simeq \exp\{-\beta[S(x_m) + h(x_m, x') - S(x')]\} \left[\frac{2\pi}{\beta U''(x_m)}\right]^{1/2} \tag{2.13}$$

with $x_m(x')$ satisfying

$$S'(x_m) + h_1(x_m, x') = 0 \tag{2.14}$$

Now (2.13) is supposed to hold for all x'; thus, differentiating it with respect to x' and using (2.14) gives

$$0 \simeq -\beta[h_2(x_m, x') - S'(x')] \times \exp\{-\beta[S(x_m) + h(x_m, x') - S(x')]\} \left[\frac{2\pi}{\beta U''(x_m)}\right]^{1/2} \tag{2.15}$$

where variations resulting from U'' are ignored as of higher order in $\beta^{-1/2}$. Consequently,

$$h_2(x_m, x') - S'(x') = 0 \tag{2.16}$$

Combining (2.14) and (2.16) leads to

$$S(x_m) + h(x_m, x') - S(x') \simeq \text{const} =: w \tag{2.17}$$

Thus

$$\mu \simeq \exp(-\beta w)\left[\frac{2\pi}{\beta\langle U''(x)\rangle}\right]^{1/2} \tag{2.18}$$

taking the average in some sense, and finally,

$$z_X \simeq -\beta w + \frac{1}{2}\log\frac{2\pi}{\beta\langle U''(x)\rangle} \tag{2.19}$$

This turns out not to be useful, however, partly because the meaning of $\langle U''(x)\rangle$ is not clear. Nonetheless, a variant of this method, namely a renormalization scheme for understanding the asymptotic behavior of a sequence of powers L^{q_n}, will be used to great effect in Section 5.

An alternative way to evaluate (2.7), which is used in Sections 3 and 4, is to rewrite it as

$$Z_{N,X} = \int \exp[-\beta W_N(\mathbf{x})] \prod dx_n \tag{2.20}$$

where

$$W_N(\mathbf{x}) = \sum_{n=0}^{N-1} h(x_n, x_{n+1}) \tag{2.21}$$

It can be treated for large β by the multidimensional saddle-point method, yielding

$$Z_{N,X} \simeq \sum \exp[-\beta W_N(\mathbf{x})]\,(2\pi/\beta)^{N/2}\,(\det D^2 W_N)^{-1/2} \tag{2.22}$$

where the sum is taken over all local minima of W_N (in some circumstances the lowest minimum may suffice). Now

$$\log \det D^2 W_N \simeq N(\chi + \tau) \tag{2.23}$$

(the Thouless formula[21]), where χ is the Lyapunov exponent of the corresponding orbit segment and

$$\tau = \langle \log[-h_{12}(x, x')] \rangle \tag{2.24}$$

the average being taken along the sequence. Thus

$$z_X \simeq z_* + \tfrac{1}{2}\log(2\pi/\beta) - \tfrac{1}{2}(\langle \chi \rangle + \langle \tau \rangle) \tag{2.25}$$

where

$$z_* = \lim_{N \to \infty} N^{-1} \log Z_{N,*} \tag{2.26}$$

with

$$Z_{N,*} = \sum \exp[-\beta W_N(\mathbf{x})] \tag{2.27}$$

and the averages in (2.25) are weighted over the minima in proportion to their contribution to $Z_{N,*}$.

3. THE INTEGRABLE REGIME

3.1. Integrable Systems

A Frenkel–Kontorova model (1.1) is said to be *integrable* if its zero-temperature equilibrium states are the uniformly spaced sequences

$$x_n = n\rho + \theta, \qquad \theta, \rho \text{ arbitrary} \tag{3.1}$$

This is equivalent (see Appendix) to the generating function h having the special form

$$h(x, x') = F(x' - x) - S(x') + S(x) \tag{3.2}$$

for some functions F and S with $F'' > 0$ and S periodic of period 1. Since the generating function enters the partition function (2.2) only as a sum along sequences, the contribution of S in (3.2) telescopes and so we can ignore it [mathematically, $S(x') - S(x)$ is a *coboundary* and $h(x, x')$ is *cohomologous* to $F(x' - x)$].

Taking segments $x_0, ..., x_N$ with free ends and regarding configurations $x_0, ..., x_N$ and $x_0+1, ..., x_N+1$ as equivalent, we obtain

$$z_X = \log \int \exp[-\beta F(\xi)]\, d\xi \tag{3.3}$$

For the special case $F(\xi) = \frac{1}{2}\xi^2$ this can be integrated explicitly to

$$z_X = \frac{1}{2} \log \frac{2\pi}{\beta} \tag{3.4}$$

giving a configuration space contribution of $\frac{1}{2}T$ to the energy e and hence of $\frac{1}{2}$ to the specific heat C_P. Of course, momentum-space contributions of $\frac{1}{2}T$ and $\frac{1}{2}$ from (2.6) also need adding to e and C_P, respectively.

For general integrable systems, the integral (3.3) can be approximated at low temperature by the saddle-point method, yielding

$$z_X = -\beta F(\xi) + \frac{1}{2} \log \frac{2\pi}{\beta F''(\xi)} + O(\beta^{-1/2}) \tag{3.5}$$

where ξ is the minimum of F. This gives specific heat $C_P = \frac{1}{2} + O(T^{1/2})$.

If an external pressure is applied, then

$$h(x, x') = F(x' - x) + P(x' - x) \tag{3.6}$$

and the minimizing ξ depends on P as follows:

$$F'(\xi) = -P \tag{3.7}$$

So

$$z_X = -\beta(F(\xi) + P\xi) + \frac{1}{2} \log \frac{2\pi}{\beta F''(\xi)} + O(\beta^{-1/2}) \tag{3.8}$$

For the special case $F = \frac{1}{2}\xi^2$, we obtain

$$z_X = -\frac{1}{2}\beta P^2 + \frac{1}{2} \log \frac{2\pi}{\beta} \tag{3.9}$$

and so the mean spacing is $\rho = -\beta^{-1}\, \partial z/\partial P = -P$, and the compressibility is $\kappa = -\partial \rho/\partial P = 1$.

For the general integrable system with pressure, (3.7) implies that

$$\partial \xi/\partial P = -1/F''(\xi) \tag{3.9a}$$

Then using (3.8), the mean spacing comes out to be

$$\rho = \xi - F'''(\xi)/2\beta + O(\beta^{-3/2}) \tag{3.10}$$

Note that we obtain compressibility

$$\kappa = -\partial\rho/\partial P = 1/F''(\xi) + O(T) \tag{3.11}$$

and thermal expansion

$$\partial\rho/\partial T = -\tfrac{1}{2}F'''(\xi) + O(T^{1/2}) \tag{3.12}$$

3.2. Systems Close to Integrable

If h is close to integrable, e.g.,

$$h(x, x') = F(x' - x) + P(x' - x) + \lambda V(x, x') \tag{3.13}$$

with λ small, then KAM theory (e.g., ref. 1), translated into this context, shows that with large probability in the pressure P, the ground states have the form

$$x_n = X(n\rho + \theta) \tag{3.14}$$

for some irrational ρ and smooth function X, depending on P and λ. Then the partition function is dominated at low temperatures by the circle of ground states formed from (3.14) by letting θ vary.

Now define $E(\xi)$ to be the mean energy per site for the minimum-energy states of mean spacing ξ with P fixed at zero. This was shown by Aubry[3] to be a strictly convex function of ξ. At zero temperature, the effect of pressure P is to select the mean spacing ξ which minimizes

$$w(\xi) = E(\xi) + P\xi \tag{3.15}$$

Then the leading-order contribution to the energy (1.1) is $Nw(\xi)$. In fact, the deviation of the energy from this in a ground state can be shown to be just a coboundary (by the theory of dynamic programming; e.g., ref. 7).

Next we have to estimate the integral in the partition function. For low temperature the dominant contribution can be obtained by expanding the energy to second order. Since θ is arbitrary, the second variation D^2W of the energy is degenerate, but the range of integration is bounded in the θ direction ($\int d\theta = 1$), so it is enough to consider transverse variations. D^2W is positive definite with respect to transverse variations because (i) the ground state is a minimum-energy state with respect to variations fixing the

ends (and by ref. 16 this implies a nondegenerate minimum), and (ii) it is a nondegenerate minimum with respect to a change of mean spacing (by strict convexity of E). Rather than calculate the determinant of D^2W for transverse variations, we take a short cut, namely, we modify the boundary conditions so that variations in x_0 and x_N are in antiphase. As is standard in statistical mechanics, this may make a significant change to the partition function, but after taking the logarithm, dividing by N, and taking the limit as N goes to infinity, the change disappears. The determinant for variations with antiphase boundary conditions is easily computed to be

$$\det D^2W = 4 \prod [-h_{12}(x_n, x_{n+1})] \tag{3.16}$$

adapting ref. 25 and using the fact that the determinant for in-phase boundary conditions is (essentially) zero (the only contribution comes from the coboundary mentioned above). Following the notation of (2.24), we write this as

$$\det D^2W = 4 \exp N\tau \tag{3.17}$$

Hence

$$\begin{aligned} Z_{N,X} &\simeq \exp(-\beta N w)\,(2\pi/\beta)^{N/2}\,(\det D^2 W_n)^{-1/2} \\ &= 4 \exp(-\beta N w - \tfrac{1}{2} N\tau)\,(2\pi/\beta)^{N/2} \end{aligned} \tag{3.18}$$

leading to

$$z_X \simeq -\beta w(\xi) - \frac{1}{2}\tau + \frac{1}{2}\log\frac{2\pi}{\beta} \tag{3.19}$$

This gives specific heat 1/2 as before, but the pressure dependence is more interesting. First note from (3.15) that ξ is determined as a function of P by

$$E'(\xi) = -P \tag{3.20}$$

and hence

$$\partial\xi/\partial P = -1/E''(\xi) \tag{3.21}$$

Using (3.20) and (3.21), we find that the mean spacing is

$$\rho = -\beta^{-1}\,\partial z/\partial P = \xi - \frac{\tau'(\xi)}{2\beta E''(\xi)} \tag{3.22}$$

In particular, note that at low temperature, the compressibility is

$$\kappa = -\partial\rho/\partial P = -\xi'(P) = 1/E''(\xi) \tag{3.23}$$

a result which makes eminent sense, as this is the zero-temperature result.[3] More interestingly, note that the leading-order thermal expansion is given by

$$\partial\rho/\partial T = -\tfrac{1}{2}\tau'(\xi)/E''(\xi) \tag{3.24}$$

For an integrable system, it is easily shown that

$$\exp \tau(\xi) = E''(\xi) \tag{3.25}$$

and so (3.24) reduces to $-\frac{1}{2}E'''(\xi)$, agreeing with (3.12). But (3.24) is the general near-integrable result.

If the pressure P is in the set of small probability for which KAM theory does not apply, then strictly speaking this counts as being in the anti-integrable regime. Nonetheless, a simple treatment will be sketched here of the most important case, namely when the minimizing mean spacing is a low-order rational p/q. If T is sufficiently small, then the partition function is dominated by the minimizing periodic state of mean spacing p/q. Then, using (2.22), we obtain

$$z_X = -\beta w + \frac{1}{2}\log\frac{2\pi}{\beta} - \frac{1}{2}(\chi + \tau) \tag{3.26}$$

where w is the mean energy per site for the minimizing state, χ is its Lyapunov exponent, and τ is given by (2.24). For the model (1.8), then $\tau = 0$ and

$$\chi \simeq C_{pq}\lambda^q \tag{3.27}$$

for some constant C_{pq}.[9] The approach of ref. 14 shows that

$$w = \frac{1}{2}\left(\frac{p}{q} - a\right)^2 + \mathcal{O}(\lambda) \tag{3.28}$$

Then from (3.26),

$$z_X \simeq -\beta\left[\frac{1}{2}\left(\frac{p}{q} - a\right)^2 + \mathcal{O}(\lambda)\right] + \frac{1}{2}\log\frac{2\pi}{\beta} - \frac{1}{2}C_{pq}\lambda^q \tag{3.29}$$

[3] Incidentally, using ref. 8, it can easily be shown that $E''(\xi)$ has the dynamical systems interpretation of the reciprocal of the "torsion" of the invariant circle of rotation number ξ (see ref. 10 for a definition).

This leads via (2.3) and (2.4) to configuration-space contributions

$$e \simeq \frac{1}{2}\left(\frac{p}{q} - a\right)^2 + \mathcal{O}(\lambda) + \frac{1}{2}T \tag{3.30}$$

$$C_P = \frac{1}{2} \tag{3.31}$$

and via (2.5) to

$$\rho = p/q + \mathcal{O}(\lambda) \tag{3.32}$$

More detailed analysis might be expected to reveal the opening up of a tongue of width of order λ^q in which ρ is very close to p/q, for $T \ll \lambda^q$.

A referee raised a question about connections with continuum system

$$H[p, u] = \int \tfrac{1}{2}p^2(x) + \tfrac{1}{2}u'(x)^2 + V(u(x))\,dx \tag{3.33}$$

whose statistical mechanics was studied, for example, in refs. 18 and 22. This system can be obtained from the Frenkel–Kontorova model

$$H = \sum \tfrac{1}{2}p_n^2/m + \tfrac{1}{2}t(u_{n+1} - u_n)^2 + \lambda V(u_n) \tag{3.34}$$

in the scaling limit $t = m = 1/\lambda$, $\lambda \to 0$, on putting $x = n\lambda$. It gives a good way of studying the Frenkel–Kontorova model for small λ when the minimizing mean spacing is an integer or nearly so. Probably the neighborhood of any rational p/q could be treated by first deriving a suitable single-resonance model (e.g., as in ref. 14) and then using the continuum approximation for λ^q small enough, but I have not pursued this.

4. THE ANTI-INTEGRABLE REGIME

For the presentation of this section, we specialize to models of the form (1.4), but allowing the potential to be replaced by an arbitrary function V with one minimum per period. The parameter a is used instead of the pressure $P = -at$. Near the anti-integrable limit ($t = 0$), we scale λ to 1.

4.1. The Anti-Integrable Limit

At the anti-integrable limit

$$h(x, x') = V(x) \tag{4.1}$$

Hence

$$Z_{N,X} = \int \exp\left[-\beta \sum V(x_n)\right] \prod dx_n \tag{4.2}$$

This is dominated by the minimizing states, which are simply given by choosing $x_n = x_{\min} + m_n$, for any sequence of integers m_n, where $x_{\min}$ is the minimum of V in $[0,1)$, say. Each anti-integrable minimizing state contributes

$$\left(\frac{2\pi}{\beta V_m''}\right)^{N/2} \tag{4.3}$$

to $Z_{N,X}$, where $V_m'' = V''(x_{\min})$. A problem is that there are infinitely many minimizing states even for N fixed. If we restrict $(x_n)_{n=0\ldots N}$ to a box of size Nv, some v, then there are $(Nv)^N$ of them. This leads to

$$Z_{N,X} \simeq \left(\frac{2\pi}{\beta V_m''}\right)^{N/2} (Nv)^N \tag{4.4}$$

As for an ideal gas, we regard the x_n as indistinguishable, which divides out the N^N term, and we obtain

$$z_X = \frac{1}{2} \log \frac{2\pi}{\beta V_m''} + \log v \tag{4.4}$$

This leads to configuration-space contributions $e = \frac{1}{2}T$ and $C_P = \frac{1}{2}$ (to which the usual momentum-space contributions should be added as in Section 3). Equation (2.5) cannot be used to obtain ρ, because $t = 0$, and since the x_n are indistinguishable, the concept of mean spacing $\langle x_{n+1} - x_n \rangle$ does not make much sense anyway.

4.2. Near the Anti-Integrable Limit

Near the anti-integrable limit, we take

$$h(x, x') = V(x) + \tfrac{1}{2}t(x' - x - a)^2 \tag{4.6}$$

More general forms of perturbation to the anti-integrable limit could be considered, but this one suffices to give the ideas.

Then each of the minimizing states $(x_n)_{n \in \mathbb{Z}}$ with

$$t\,|x_{n+1} - 2x_n + x_{n-1}| \ll V_m'' \tag{4.7}$$

has a unique continuation $(\tilde{x}_n)$,[4] with

$$\tilde{x}_n \simeq x_n - t(x_{n+1} - 2x_n + x_{n-1})/V_m'' \tag{4.8}$$

The energy of a segment 0, ..., N increases by

$$\sum_{n=0}^{N-1} \tfrac{1}{2}t(x_{n+1}-x_n-a)^2 \tag{4.9}$$

to first order in t.

Let us assume for the rest of this section that the temperature is low enough that

$$tT \ll (V_m'')^2 \qquad \text{and} \qquad T \ll V_{\max} - V_{\min} \tag{4.10}$$

where $V_{\max}$ and $V_{\min}$ denote the maximum and minimum values of V. Then $Z_{N,\chi}$ is dominated by these local minima, and we can use formula (2.25), with $\chi = \log V_m''$, $\tau = 0$, and

$$Z_{N,*} \simeq \exp(-\beta N V_{\min}) \sum_{(\delta_n)} \exp\left[-\frac{1}{2}\beta t \sum_{n=0}^{N-1} (\delta_n - a)^2\right] \tag{4.11}$$

where the sum is over sequences of integers $\delta_n = m_{n+1} - m_n$. It is not necessary to restrict ourselves to sequences satisfying condition (4.7), because by (4.10) the difference is exponentially small.

Equation (4.11) can be rewritten as

$$Z_{N,*} \simeq e^{-\beta N V_{\min}} \Theta(\beta t, a)^N \tag{4.12}$$

where

$$\Theta(\tau, a) = \sum_{\delta \in Z} e^{-\tau(\delta - a)^2/2} \tag{4.13}$$

So

$$z_* \sim -\beta V_{\min} + \log \Theta(\beta t, a) \tag{4.14}$$

The function Θ is a famous one which appears in the analysis of Riemann's zeta function (e.g., ref. 11). It has the following behavior, as can be easily proved. For τ large

$$\Theta(\tau, a) \sim 2 \cosh \tfrac{1}{2}\tau\varepsilon \, e^{-\tau\varepsilon^2/2} e^{-\tau/8} \tag{4.15}$$

where

$$\varepsilon = \tfrac{1}{2} - \{a\} \tag{4.16}$$

and $\{a\}$ is the distance from a to the nearest integer $[a]$. When $\tau\varepsilon \gg 1$ this reduces to

$$\Theta(\tau, a) \sim e^{-\tau\{a\}^2/2} \tag{4.17}$$

For τ small,

$$\Theta(\tau, a) \sim \left(\frac{2\pi}{\tau}\right)^{1/2} \tag{4.18}$$

The term $\beta V_{\min}$ in (4.14) is not important, as it does not contribute to the specific heat nor to the mean spacing, so we will leave it out. The second term in (4.14) contributes

$$\begin{cases} -\frac{1}{2}\beta t\{a\}^2 & \text{if} \quad \beta t\varepsilon \gg 1 \\ -\frac{\beta t}{8} - \frac{1}{2}\beta t\varepsilon^2 + \log\left(2\cosh\frac{1}{2}\beta t\varepsilon\right) & \text{if} \quad \beta t \gg 1 \quad \text{and} \quad \varepsilon \prec \frac{1}{\beta t} \\ \frac{1}{2}\log\frac{2\pi}{\beta t} & \text{if} \quad \beta t \ll 1 \end{cases} \tag{4.19}$$

The symbol $\prec$ denotes "less than or of the same order as." Hence we obtain a contribution to the specific heat of

$$\begin{cases} 0 & \text{if} \quad T \ll t\varepsilon & \text{(4.20a)} \\ x^2 \operatorname{sech}^2 x, \quad \text{where } x = \frac{1}{2}\beta t\varepsilon, & \text{if} \quad T \ll t \quad \text{and} \quad T \succ t\varepsilon & \text{(4.20b)} \\ \frac{1}{2} & \text{if} \quad T \gg t & \text{(4.20c)} \end{cases}$$

To this should be added contributions of $\frac{1}{2}$ from the term $\frac{1}{2}\log 2\pi/\beta$ in (2.25) and $\frac{1}{2}$ from the momentum integral (2.6). The enhanced specific heat (4.20b) for $T \sim t\varepsilon$, ε small, can be seen as a Schottky anomaly.[23, 24] Calculation to higher order in t would be expected to reveal further Schottky anomalies. Instead of doing this, I will use a renormalization procedure in Section 5 to deduce an infinite sequence of Schottky anomalies as the temperature is reduced. This is a rigorous version of the renormalization of refs. 23 and 24, which used two approximations: (i) approximation of the Frenkel–Kontorova model by a spin model, (ii) neglect of nonrenormalizable spin configurations.

The existence of a regime (4.20) where the specific heat is 3/2, viz. $T \gg t$, is a new phenomenon, to my knowledge, though not particularly surprising. It can be understood heuristically on the basis of the growth of the number of anti-integrable equilibrium states with respect to energy.

The mean spacing can also be found from (4.14) and the analog of (2.5) for parameter a:

$$\rho = a - \frac{1}{\beta t}\frac{\partial z}{\partial a} \tag{4.21}$$

$$\rho \sim \begin{cases} [a] & \text{if} \quad T \ll t\varepsilon \\ M + \frac{1}{2}\left[1 + \tanh \beta t \left(a - M - \frac{1}{2}\right)\right], & \text{if} \quad a \approx M + \frac{1}{2} \quad \text{and} \quad T \ll t \\ a & \text{if} \quad T \gg t \end{cases} \tag{4.22}$$

5. THE TRANSITION REGIME

At $T=0$, there is a qualitative transition in the ground state across a certain fractal "curve" in the (k, P) plane. Below the curve, there is a circle of ground states, so they have a phason. Above the curve, the ground state has phonon gap. Many features of the transition can be understood by renormalization.[13] I recall the scheme rapidly. It is easiest to describe if we assume that we know a ground state $(x_n)_{n \in \mathbb{Z}}$.

Suppose we know that the mean spacing ρ of the ground state occurs between the integers K and $K+1$. Then if the bond from x_n to x_{n+1} crosses $K+1$ maxima of the potential, label it by υ, and if it crosses K maxima, label it by τ. Since the ground state is rotationally ordered (i.e., $x_n \bmod \mathbb{Z}$ are in the same order on the circle as $n\rho \bmod \mathbb{Z}$), these are the only two possibilities. By defining

$$\begin{aligned} \upsilon(x, x') &= h(x, x' + K) \\ \tau(x, x') &= h(x, x' + K + 1) \end{aligned} \tag{5.1}$$

and subtracting appropriate integers from the x_n, the ground state reduces to a ground state of a model with two types of interaction (υ and τ), for which the x_n remain in an interval about 0, and $x_n \leqslant 0 < x_{n+1}$ for each υ-bond, $x_{n+1} \leqslant 0 < x_n$ for each τ-bond. By rotational order, either every υ-bond is surrounded by τ-bonds or every τ-bond is surrounded by υ-bonds. Let us suppose the first case. Then we can eliminate the site at the right hand end of each υ-bond by defining

$$\begin{aligned} \tilde{\upsilon}(x, x') &= \min_z \left(\upsilon(x, z) + \tau(z, x')\right) \\ \tilde{\tau}(x, x') &= \tau(x, x') \end{aligned} \tag{5.2}$$

to obtain a new chain with two interactions ($\tilde{\upsilon}$ and $\tilde{\tau}$), and an equivalent ground state. In the second case, eliminate the sites at the right-hand end of every τ-bond in the same way.

It is convenient to rescale the configuration space and the scale of energy

$$\begin{aligned} \bar{\upsilon}(x, x') &= J\tilde{\upsilon}(x/\alpha, x'/\alpha) \\ \bar{\tau}(x, x') &= J\tilde{\tau}(x/\alpha, x'/\alpha) \end{aligned} \tag{5.3}$$

by numbers J and α, in order to try to make the new pair $(\bar{v}, \bar{\tau})$ look as much like (v, τ) as possible, by enforcing some normalization conditions [in fact, it is also useful to perform some additional changes to $(\bar{v}, \bar{\tau})$ which do not change the ground states].

The transformation R: $(v, \tau) \mapsto (\bar{v}, \bar{\tau})$ is called "renormalization." The remarkable numerical observation is that R possesses a hyperbolic invariant set C of the form $\{(v_\rho^*, \tau_\rho^*)$: ρ Diophantine irrational $\in (0, 1)\}$, with two-dimensional unstable manifolds.[17] [4] The parameter ρ labels the mean spacing of the ground state. The two unstable directions correspond to (i) the sliding–pinned transition and (ii) change of pressure (which changes the mean spacing of the ground state). We will denote displacements in these two directions by Δk and ΔP, respectively. At the "golden point" where $\rho = \gamma^{-1}$, $\gamma = \frac{1}{2}(1 + \sqrt{5})$, which is a fixed point[5] of renormalization in C, the numbers J and α are $J \simeq 4.339143904$ and $\alpha \simeq -1.4148360$, and the expansions in the two directions are $\delta \simeq 1.6279500$ and $\eta = -J/\gamma \simeq -2.6817384$, respectively.[13]

An analogous renormalization R' can easily be defined for nonzero temperature, and this is the main novelty of this paper. Instead of minimizing the energy with respect to certain sites, we integrate out certain sites in the partition function. Thus the analog of (5.2) is

$$\begin{aligned} \tilde{v}(x, x') &= -T \log \int dz\, e^{-(v(x, z) + \tau(z, x'))/T} \\ \tilde{\tau}(x, x') &= \tau(x, x') \end{aligned} \tag{5.4}$$

and the renormalization R' is defined by composing (5.4) with (5.3). The effect of the scale change J in (5.3) is to increase the temperature by a factor J.

To unify the $T = 0$ and $T > 0$ cases, we note that: (i) if v, τ, and T are multiplied by the same positive number λ, then $\tilde{v}$ in (5.4) is simply multiplied by λ, and (ii) (5.2) is the $T \to 0$ limit of (5.4), because

$$\kappa(x, x') := v_{22}(x, z) + \tau_{11}(z, x') \tag{5.4a}$$

is positive at the minima.

[4] Strictly speaking, the scheme described in ref. 17 does not apply directly here. The scheme of ref. 17 searches for a minimum-energy state of given mean spacing, whereas here we want to find the ground state, whose mean spacing is not necessarily known in advance. However, the modifications required are simple and lead to the above conclusions.

[5] Actually it is a period-2 cycle of R, but a symmetry (interchange of v and τ) can be used to reduce it to a fixed point.

Hence we can think of the renormalization R' as acting in the subset with $T \geqslant 0$ of the projective space M of equivalence classes of triples (v, τ, T) under the equivalence relation $(v, \tau, T) \sim (\lambda v, \lambda\tau, \lambda T)$, for all $\lambda > 0$. It has the invariant set C on the boundary $T = 0$. The only effect of the enlargement of the space to include $T > 0$ is to add one further unstable direction, with expansion rate J, into $T > 0$.

Let us describe some of the consequences of the existence of the hyperbolic invariant set C. It is simplest to describe in the neighborhood of the golden point, because this is a fixed point of renormalization, whereas the general orbit on C is aperiodic. The renormalization picture implies that when we integrate over the sites to be eliminated, near the golden point, the partition function $Z_{F_m, X}$ for a segment of length F_m (the mth Fibonacci number) satisfies

$$Z_{F_m, X}(\beta, \Delta P, \Delta k) \sim Z_{F_{m-1}, X}\left(\frac{\beta}{J}, \eta\, \Delta P, \delta\, \Delta k\right) \alpha^{-F_{m-1}} \left(\frac{2\pi}{\beta\kappa}\right)^{(F_m - F_{m-1})/2} \tag{5.5}$$

where κ denotes the geometric mean of the values of (5.4a) over the eliminated sites. The way κ scales with m is subtle, being related to the scaling for the phonon gap,[13] but it does not depend on β and so is irrelevant for the computation of the specific heat, so we will suppress its dependence on ΔP and Δk for the moment. It follows that $z_X(\beta, \Delta P, \Delta k)$ scales like

$$z_X(\beta, \Delta P, \Delta k) \sim \gamma^{-1} z_X\left(\frac{\beta}{J}, \eta\, \Delta P, \delta\, \Delta k\right) - \gamma^{-1} \log \alpha + (1 - \gamma^{-1}) \log \left(\frac{2\pi}{\beta\kappa}\right)^{1/2} \tag{5.6}$$

because $F_m \sim \gamma F_{m-1}$. By (2.3) we obtain

$$\tilde{e}(T, \Delta P, \Delta k) \sim \frac{1}{\gamma J} \tilde{e}(JT, \eta\, \Delta P, \delta\, \Delta k) \tag{5.7}$$

where

$$\tilde{e} = -\partial z_X / \partial \beta - \tfrac{1}{2} T \tag{5.8}$$

and so by (2.4) the contribution to the specific heat from $\tilde{e}$ scales like

$$C_P(T, \Delta P, \Delta k) \sim \gamma^{-1} C_P(JT, \eta\, \Delta P, \delta\, \Delta k) \tag{5.9}$$

In particular, this says that at $\Delta p = \Delta k = 0$,

$$C_P(T) \sim T^{\log \gamma / \log J} c(\log T) \tag{5.10}$$

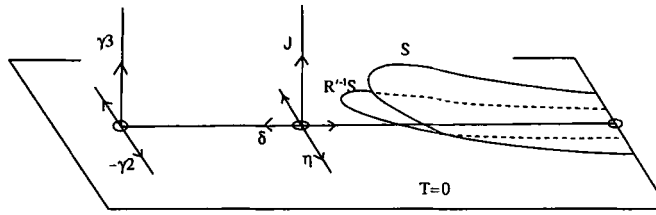

Fig. 1. Sketch of the action of renormalization R' on the space M, showing three invariant sets lying in the surface $T=0$, represented by points, and a surface S around which a Schottky anomaly occurs, plus one of its preimages.

where c is a function of period $\log J$. Of course, one has to add to this the contribution $\frac{1}{2}$ from the $\frac{1}{2}T$ in (5.8) and the $\frac{1}{2}$ from the momentum integral (2.6), but since $\log \gamma/\log J \simeq 0.32787 < 1$, (5.10) is the dominant term at low temperature.

For the scaling of ρ, we first argue that because of the procedure at the beginning of this section of subtracting integers from the x_n, the formula (2.5) should be interpreted as giving the deviation $\Delta\rho$ of the mean spacing from that corresponding to the reference ground state. Then from (5.6), ignoring (possibly incorrectly) the dependence of κ on ΔP, we obtain

$$\Delta\rho(T, \Delta P, \Delta k) \sim -\gamma^{-2}\, \Delta\rho(JT, \eta\, \Delta P, \delta\, \Delta k) \tag{5.11}$$

In particular, taking the limit $T \to 0$ leads to

$$\Delta\rho \sim \Delta P^{\log \gamma^2/\log |\eta|} \tag{5.12}$$

The exponent is 0.975628. This agrees with the $T=0$ result of ref. 13.

The renormalization scheme R' is not limited to the transition regime. There is a set of integrable systems which is invariant under renormalization and set of anti-integrable systems which is invariant under renormalization. I believe that these connect up as indicated in Fig. 1. Hence renormalization can say things about the intermediate regimes, too.

In particular, the renormalization scheme provides a rigorous foundation for the phenomenon of hierarchical melting of incommensurate structures in the pinned regime, studied in refs. 23, 24, and 19. In Section 4 we found one Schottky anomaly at around $T \simeq (\frac{1}{2} - \{a\})t$. Generalizing to the function space M, we expect a Schottky anomaly around a codimension-1 surface S as indicated in Fig. 1. By inverse renormalizing, we deduce an infinite sequence of Schottky anomalies around the surface $(R')^{-k}S$, $k = 0, 1, 2, \ldots$.

6. DISCUSSION

Low-temperature scaling laws have been derived for the free energy, specific heat, and mean spacing in classical Frenkel–Kontorova models, in the integrable, anti-integrable, and transition regions of parameter space. One of the interesting discoveries is of a regime $t \ll T \ll 1$ in which the specific heat is enhanced from 1 to 3/2. Another interesting result is the extension of the renormalization scheme of ref. 13 to nonzero temperature and the resulting nontrivial scaling laws like (5.10) near the sliding–pinned transition and associated results like hierarchical melting in the pinned regime.

One natural question is where the effects of "discrete breathers" show up; these are self-localized periodic solutions whose existence is proved in ref. 15. Presumably they affect the time correlations.

A next step could be to extend these results to quantum mechanical Frenkel–Kontorova models for small Planck constant. For example, suppression of the phonons with frequency ω such that $\hbar\omega \geqslant T$ is to be expected.

APPENDIX

Theorem. A Frenkel–Kontorova model is integrable iff its generating function has the form

$$h(x, x') = F(x' - x) - S(x') + S(x) \tag{A.1}$$

for some functions F and S with $F'' > 0$ and S of period 1.

Proof. If h has this form, then its equilibrium states are the solutions of

$$F'(x_n - x_{n-1}) - S'(x_n) - F'(x_{n+1} - x_n) + S'(x_n) = 0 \tag{A.2}$$

so $x_{n+1} - x_n = \text{const}$, since F' is monotone. So the equilibrium states are the sequences

$$x_n = n\rho + \theta \tag{A.3}$$

which we took as our definition of integrability in Section 3.

Conversely, suppose the equilibrium states are the sequences (A.3) with Θ and ρ arbitrary. Then

$$h_2(\theta - \rho, \theta) + h_1(\theta, \theta + \rho) = 0 \tag{A.4}$$

Differentiating with respect to ρ, we obtain

$$h_{12}(\theta-\rho,\theta)=h_{12}(\theta,\theta+\rho) \tag{A.5}$$

If ρ is irrational, then density of the orbit of rotation by ρ and continuity of h_{12} imply that $h_{12}(\theta,\theta+\rho)$ is independent of θ. Since the irrationals are dense in the reals, continuity implies the same for rational ρ. Hence

$$h_{12}(\theta,\theta+\rho)=f(\rho) \tag{A.6}$$

a function of ρ only.

Now integrate h_{12} over the triangle with vertices (x,x'), (x,x), (x',x') in two ways to obtain

$$\int_0^{x'-x}(x'-x-\rho)\,f(\rho)\,d\rho=h(x',x')-h(x,x')-s(x')+s(x) \tag{A.7}$$

where

$$s(x)=\int_0^x h_1(y,y)\,dy \tag{A.8}$$

Let

$$S(x)=s(x)-s(1)x \tag{A.9}$$

Then S is periodic of period 1. Now

$$dh(x',x')/dx'=h_1(x',x')+h_2(x',x')=0 \tag{A.10}$$

[compare the case $\rho=0$ of (A.4)]. So

$$h(x',x')=K,\quad \text{const} \tag{A.11}$$

Let

$$F(u)=K-\int_0^u(u-\rho)\,f(\rho)\,d\rho-s(1)u \tag{A.12}$$

By differentiating twice, $F''(u)=-f(u)>0$. Furthermore, rearranging (A.7) yields

$$h(x,x')=F(x'-x)-S(x')+S(x) \tag{A.13}$$

ACKNOWLEDGMENTS

I am grateful to Serge Aubry for discussions about his papers on this topic. This work was supported by the Nuffield Foundation, the British Council Alliance scheme, an EC network on "Nonlinear Approach to Coherent and Fluctuating Phenomena in Condensed Matter and Optical Physics," and the U.K. Science and Engineering Research Council. The bulk was completed during a visit to the Institut des Hautes Etudes Scientifiques in April 1994, which I thank for its hospitality.

REFERENCES

1. V. I. Arnol'd, *Mathematical Methods of Classical Mechanics* (Springer, Berlin, 1978, 1989).
2. S. Aubry, A unified approach to the interpretation of displacive and order–disorder systems I: Thermodynamical aspect, *J. Chem. Phys.* **62**:3217–3229 (1975).
3. S. Aubry, The devil's staircase transformation in incommensurate lattices, in *The Riemann Problem, Complete Integrability and Arithmetic Applications*, D. Chudnovsky and G. Chudnovsky, eds. (Springer, Berlin, 1982), pp. 221–245.
4. S. Aubry, and G. Abramovici, Chaotic trajectories in the standard map: The concept of anti-integrability, *Physica D* **43**:199–219 (1990).
5. S. Aubry and P. Y. Le Daeron, The discrete Frenkel–Kontorova model and its extensions I: exact results for the ground state, *Physica D* **8**:381–422 (1983).
6. R. Balescu, *Equilibrium and Non-Equilibrium Statistical Mechanics* (Wiley, New York, 1975).
7. D. A. Carlson, A. B. Haurie, and Leizarowitz, *Infinite Horizon Optimal Control* (Springer, Berlin, 1991).
8. Q. Chen, Area as a devil's staircase in twist maps, *Phys. Lett. A.* **123**:444–450 (1987).
9. J. M. Greene, A method for computing the stochastic transition, *J. Math. Phys.* **20**:1183–1201 (1979).
10. M. R. Herman, Dynamics connected with indefinite normal torsion, Preprint Ecole Polytechnique (Oct 1990).
11. A. Karatsuba and S. M. Voronin, *Riemann's Zeta Function* (de Gruyter, 1992).
12. V. F. Lazutkin and D. Ya. Terman, Percival variational principle for invariant measures and commensurate–incommensurate phase transitions in one-dimensional chains, *Commun. Math. Phys.* **94**:511–522 (1984).
13. R. S. MacKay, Scaling exponents at the transition by breaking of analyticity for incommensurate structures, *Physica D* **50**:71–79 (1991).
14. R. S. MacKay Greene's residue criterion, *Nonlinearity* **5**:161–187 (1992).
15. R. S. MacKay and S. Aubry, Existence of breathers for time-reversible or Hamiltonian networks of weakly coupled oscillators, *Nonlinearity* **7**:1623–1643 (1994).
16. R. S. MacKay and I. C. Percival, Converse KAM theory: Theory and practice, *Commun. Math. Phys.* **98**:469–512 (1985).
17. R. S. MacKay and J. Stark, Locally most robust circles and boundary circles for area-preserving maps, *Nonlinearity* **5**:867–888 (1982).
18. Y. Okwamoto, H. Takayama, and H. Shiba, Incommensurate–commensurate crossover in generalized one-dimensional Ginzburg–Landau fields, *J. Phys. Soc. Japan* **46**:1420–1427 (1979).

19. R. Schilling and S. Aubry, The static structure factor of one-dimensional non-analytic incommensurate structures, *J. Phys. C* **20**:4881–4889 (1987).
20. Ya. G. Sinai, Commensurate–incommensurate phase transitions in one-dimensional chains, *J. Stat. Phys.* **29**:401–425 (1982).
21. D. J. Thouless, A relation between the density of states and range of localization for one-dimensional random systems, *J. Phys. C* **5**:77–81 (1972).
22. L. A. Turkevich and S. Doniach, *Ann. Phys.* **139**:343–418 (1982).
23. F. Vallet, R. Schilling, and S. Aubry, Hierarchical low-temperature behaviour of one-dimensional incommensurate structures, *Europhys. Lett* **2**:815–822 (1986).
24. F. Vallet, R. Schilling, and S. Aubry, Low-temperature excitations, specific heat and hierarchical melting of a one-dimensional incommensurate structure, *J. Phys. C* **21**: 67–105 (1988).
25. R. S. MacKay and J. D. Meiss, Linear stability of periodic orbits in Lagrangian systems, *Phys. Lett. A* **98**:92–94 (1983).