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The Classical Statistical Mechanics of Frenkel–Kontorova Models

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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 $(x_n)_{n \in Z}$ 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, $h: \mathbb{R}^2 \to \mathbb{R}$ is a function (called the *generating function*) with the following two properties:

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

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

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

The Frenkel–Kontorova model is the special case

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

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

$$k = \lambda / t \qquad (1.4a)$$

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

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

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

$$P = -at \qquad (1.6)$$

we can write Frenkel-Kontorova model in the form

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

with

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

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

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