# Renormalization and Quantum Scaling of Frenkel–Kontorova Models

Nuno R. Catarino*†& Robert S. MacKay‡,
Mathematics Institute, University of Warwick
Gibbet Hill Road, Coventry CV4 7AL, U.K.

8th September 2005

**Abstract**

We generalise the classical Transition by Breaking of Analyticity for the class of Frenkel–Kontorova models studied by Aubry and others to non-zero Planck's constant and temperature. This analysis is based on the study of a renormalization operator for the case of irrational mean spacing using Feynman's functional integral approach. We show how existing classical results extend to the quantum regime. In particular we extend MacKay's renormalization approach for the classical statistical mechanics to deduce scaling of low frequency effects and quantum effects. Our approach extends the phenomenon of hierarchical melting studied by Vallet, Schilling and Aubry to the quantum regime.

Keywords: Transition by breaking of analyticity; renormalization; quantum scaling; specific heat.

## 1 Introduction

The *Frenkel–Kontorova model* (FK) is a one-dimensional lattice model exhibiting incommensurate structures. It is a system of elastically coupled particles in an external periodic potential (a discrete version of the sine–Gordon model) with Lagrangian

$$L(x,\dot{x}) = \sum_{n\in\mathbb{Z}} \left\{ \frac{\dot{x}_n^2}{2} - \mathrm{v}(x_n, x_{n+1}) \right\}, \tag{1}$$

*Present address: School of Mathematical and Computer Sciences, Colin Maclaurin Building, Heriot-Watt University, Edinburgh EH14 4AS, U.K.
†e-mail: catarino@ma.hw.ac.uk
‡e-mail: mackay@maths.warwick.ac.uk

where

$$\mathrm{v}\left(x,x'\right)=\frac{1}{2}\left(x'-x\right)^2+P\left(x'-x\right)+\frac{u}{4\pi^2}\cos\left(2\pi x\right), \qquad (2)$$

with parameters $P$ ("pressure" or $-P$ as tension) and $u$ (amplitude of the onsite potential). We call successive pairs $(x_n, x_{n+1})$ *bonds* and $\mathrm{v}\left(x_n,x_{n+1}\right)$ the *(potential) energy of the bond*. Notice that in (1) and (2) the particles' mass, the elastic coupling strength and the period of the onsite potential are all scaled to one. The FK model is a particular case of the broader class of *(Generalised) Frenkel–Kontorova models* (GFK) with Lagrangian still given by (1) but the bond energy v is a generic $\mathcal{C}^2$ function satisfying

$$\mathrm{v}\left(x+1,x'+1\right)=\mathrm{v}\left(x,x'\right)$$
$$\frac{\partial^2\mathrm{v}}{\partial x\partial x'}\left(x,x'\right)\leqslant -C<0\,.$$

In the space of parameters there are two important limits. In the *integrable* limit, the bond energy, v, depends only on $(x'-x)$. For the FK model (2) the integrable limit is attained at $u=0$ and its *minimum energy configurations* (i.e. $x\in\mathbb{R}^{\mathbb{Z}}$ such that $\forall M<N, V_{M,N}\left(x\right):=\sum_{n=M}^{N-1}\mathrm{v}\left(x_n,x_{n+1}\right)$ is minimum for all variations of $x_n$ with fixed $x_M$ and $x_N$) are arrays of equally spaced particles with *mean spacing*

$$\rho:=\lim_{-M,N\to\infty}\frac{x_N-x_M}{N-M}$$

simply $-P$. In the *anti-integrable* limit [4] the onsite term dominates, which corresponds to $u\to\infty$ in (2). All particles are then in the minima of the potential and the mean spacing is the closest integer to $-P$, or any value in between the two if non-unique.

An interesting set of codimension-2 critical points occur between these two regimes, often called *Transition by Breaking of Analyticity* (TBA): in the space of parameters $(u,P)$, for each irrational $\rho$ there is a curve $P=P_\rho\left(u\right)$ of mean spacing $\rho$ containing a critical value $u_c$ (there may be more than one $u_c$ depending on the potential). The regime for $u$ less than $u_c$ is called *subcritical* (or *sliding phase*) and above $u_c$ *supercritical* (or *pinned phase*) [5] (see figure 1). For the FK model with fixed mean spacing $\rho=\gamma^{-1}$, where $\gamma=\left(1+\sqrt{5}\right)/2$ is the golden mean, the TBA is at the critical value $u_c\simeq 0.971\,635\,406$ [15]. This is the case most often studied in the literature, since it is presumed to be the highest value of $u$ at which a TBA occurs.

For the case of mean spacing $\rho=\gamma^{-1}$, relabelling the bonds v appropriately [19] as $\tau$ and $\upsilon$ results in a Fibonacci sequence of $\tau$s and $\upsilon$s where each $\upsilon$-bond is always surrounded by $\tau$-bonds. The TBA point can be viewed as a fixed point of the renormalization operator that minimises the energy of the sum of successive $\upsilon$ and

Figure 1: Sketch of the TBA along the curve of constant mean spacing $\rho = \gamma^{-1}$. The TBA point corresponding to the critical value $u_c\left(\rho = \gamma^{-1}\right)$ is labelled. For each irrational mean spacing, $\rho$, there is a similar curve at which there is a critical point at $u_c(\rho)$ (not shown in picture).

$\tau$-bonds with suitably chosen space and energy scalings, $\alpha, \mathcal{J} \in \mathbb{R}$ respectively depending on the pair $(\upsilon, \tau)$ (actually it is also necessary to subtract a constant and a quadratic coboundary but we will suppress reference to these inessential terms) [19]. The renormalization operator has a nontrivial fixed point[1] $(\bar{\upsilon}, \bar{\tau})$ with $\alpha \simeq -1.414\,836\,0$ and $\mathcal{J} \simeq 4.399\,143\,9$. This fixed point corresponds to the critical $u_c$ along the curve in $(u, P)$ for $\rho = \gamma^{-1}$, the transition point between the subcritical and supercritical regimes. It has two unstable directions: one along the curve of constant mean spacing, with eigenvalue $\delta \simeq 1.627\,950\,0$ and the other transverse to this curve in the $(u, P)$ plane (which we call the $P$ direction), with eigenvalue $\eta = -\mathcal{J}/\gamma \simeq -2.681\,738\,4$ [19, 20].

Whereas the classical ground states of Frenkel–Kontorova models have been extensively studied since the beginning of the 1980's [1, 2, 3, 5, 23] (see also the review in chapter 1 of [11], and the book [10] for several aspects of the FK model), the extension to the quantum regime of the classical Transition by Breaking of Analyticity is still not fully understood. Most of the previous studies stem from the work of Borgonovi *et al.* [8, 9], where the authors do a numerical study of FK model in the supercritical region $u > u_c$ for the case of mean spacing $\gamma^{-1}$. They introduce a 'quantum hull function' for the expected positions $\bar{x}_n$ as the extension of Aubry's hull function (see [11], section 1.2) as well as the 'quantum $g$-function' (which reduces to $\sin(2\pi\bar{x}_n)$ in the classical limit) and verify that by increasing $\hbar$ the quantum hull function becomes a smooth version of the classical hull function and that $g_n$ tends to a sawtooth-like map. Similar results have been later obtained using various numerical or a combination of analytical and numerical methods [6, 7, 17, 16].

In a recent numerical study Zhirov *et al.* [27] claim to observe a 'quantum phase transition' in the FK model at a critical value of Planck's constant between 'sliding phonon gas' and a 'pinned instanton glass'. In fact we expect that due to KAM-type of arguments, for sufficiently irrational mean spacing the phonon energy band will survive for a small perturbation of the integrable limit $u = 0$, where the interactions between phonons of different wavenumber are small. At the anti-integrable limit, on the other hand, when the dominant interaction is the onsite periodic potential, the quantum spectrum consists of sets of $N$ degenerate Bloch bands ($N$ being the total

[1] This has now been proved by Koch [18] by reformulation as a renormalization on continuous–time Hamiltonian systems and rigorous computer–assisted bounds.

number of particles) whose width is due to tunnelling or instanton effects between distinct minima of the onsite potential. As $u$ is decreased from the anti-integrable limit, the periodic potential barrier decreases and the interaction between degenerate Bloch bands increases (when compared to $u$) from zero. The degeneracy between Bloch bands corresponding to distinct particles should therefore be lifted, widening the Bloch bands. As we approach the integrable limit, $u \to 0$, these Bloch bands must merge into a unique phonon band for some non-zero value $u_c(\hbar)$ (possibly not a unique curve corresponding to merging of distinct bands). We believe that the transition observed in [27] corresponds in fact to crossing this curve(s) $u_c(\hbar)$ at which the merging of Bloch bands should occur.

In addition to the groundstates, it is physically significant to study the effect of the TBA on the low temperature statistical mechanics of FK models. This was done for the classical case in [21]. The quantum statistical mechanics of FK models was considered in a series of papers by Giachetti and Tognetti, e.g. [13, 14], but we are not aware of any work on the effects of the TBA on the quantum statistical mechanics.

The goal of this article is to study the transition above by extending the minimum energy renormalization approach in [19] to non-zero Planck's constant and temperature, which is done in section 2. This is done in a way similar to some extent to the classical non-zero temperature extension performed in [21], but whereas in the classical partition function the kinetic and potential contributions decouple, $Z = Z_P\, Z_X$, in the quantum case this is no longer true and we have to renormalize the full partition function (and not only the potential component, $Z_X$, as is [21]). Our renormalization analysis therefore requires that we take into account not only the ground states but also time-periodic solutions in order to extend the renormalization to non-zero Planck's constant. At this point we stress that although the method is analogue to the one in [21], our analysis is completely independent. In fact, our analysis is valid for the regime $\beta\hbar \gg 1$ ($\beta$ is the inverse temperature), whereas in [21] Planck's constant is zero (see also section (2.4), where the relation between both renormalizations is discussed).

Our strategy can be summarised as follows: we construct a renormalization operator, $\mathcal{R}$, which reduces to the ground state operator, $\mathcal{R}_{\text{cgs}}$, when $\hbar$ goes to zero, i.e. $\mathcal{R}|_{\hbar=0} = \mathcal{R}_{\text{cgs}}$. Then $(u, P, \ldots, \hbar = 0)$ is an invariant subspace for $\mathcal{R}$ which includes the critical fixed point of renormalization corresponding to the TBA by construction (this is illustrated in figure 2). We then transform the zero temperature results thus obtained (i.e. scaling of the trace of the kernel) into the non-zero temperature formalism for the quantum partition function. This step is straightforward, since in Feynman functional integral formulation, the partition function (21) is simply the traced kernel (4) evaluated at an imaginary time interval $T = -\mathrm{i}\,\beta\hbar$, a procedure

Figure 2: Sketch of our strategy: We define a new, quantum, renormalization operator, $\mathcal{R}$, such that when $\hbar \to 0$ we recover the classical operator $\mathcal{R}_{\text{cgs}}$ of [19] and obtain a new eigenvalue, $\kappa$, in the direction of $\hbar$ (note that the temperature direction is not show - see text for details).

sometimes called *Wick rotation*[2] [22, section 2.2]. Having obtained the scaling of the quantum partition function, our final step is to obtain the asymptotic scaling laws for the TBA critical point.

In section 2 we start by introducing the trace of the kernel and by explaining why this is the chosen physical quantity to apply our renormalization approach. We then define a decimation procedure $\oplus$ for pairs of "bond actions" by doing the trace over intermediate particles corresponding to a partial trace over the kernel and the renormalization operator $\mathcal{R}$ by composing the decimation with the appropriate scalings. The quantum eigenvalue $\kappa$ is also introduced. Next, in subsection 2.1, we show that the classical ground state renormalization, $\mathcal{R}_{\text{cgs}}$, is obtained as the limit of zero Planck's constant and frequency of quantum renormalization. In subsection 2.2 the value of the quantum eigenvalue is determined by analysing the linearised or phonon problem. In subsection 2.4 the results obtained are 'Wick rotated' to obtain the scaling laws for quantum thermal quantities, and an extension of the phenomenon of hierarchical melting studied by Vallet, Schilling and Aubry [25, 24, 26] to the quantum regime is proposed. Finally, in the last section 3 the results obtained are discussed.

# 2 Renormalization and scaling

We begin by introducing the renormalization procedure for the action of time-periodic functions of prescribed period. Consider the class of models with the following formal sum for the action

$$\mathcal{S}(x;T) = \sum_{n\in\mathbb{Z}} s(x_n, x_{n+1};T).$$

for time–periodic functions $x_n$ of period $T$, where the *bond action* $s$ is given by

$$s(x,x';T) = \int_0^T \left\{ \frac{\dot{x}^2}{2} - \mathrm{v}(x,x') \right\} dt, \tag{3}$$

[2]The Wick rotation therefore relates the quantum mechanics (i.e. dynamics) of a system to its quantum statistics, and should not be confused with the also well-known equivalence between quantum statistics of a $d$ dimensional system to the *classical* statistics of a $d+1$ dimensional system.

and v is a GFK bond potential energy. The quantum renormalization will concern the trace of the kernel which is

$$K'(T,\hbar) = \int \mathcal{D}'x \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\mathcal{S}(x;T)},$$

where the notation $\mathcal{D}'x$ means that the integration is to be performed over the space of periodic paths $x$ with period $T$ and includes the integration over the endpoints $dx(0)$ (i.e. $x(T) = x(0)$ and $\mathcal{D}'x = dx(0)\,\mathcal{D}x$).

The reasons why we consider the trace of the kernel (as opposed to the kernel itself) are twofold: 1) Our objective is generalise the renormalization to non-zero temperature and Planck's constant. Since the quantum partition function is simply the 'Wick rotated' version of $K'$, given by equation (21), the analysis of the real-time (i.e. zero temperature) renormalization operator (6) is readily transformed into an imaginary-time (i.e. non-zero temperature) renormalization (22). 2) For technical reasons (which will become clear in subsection 2.2) we need to restrict to time-periodic functions to be able to obtain the scaling laws (20–26). This last point is not a big limitation for zero temperature quantum mechanics because quantum averages of observables (e.g. correlation functions) could be obtained from derivatives of $\ln K'$ with respect to source terms if the appropriate eigenvalues of $\mathcal{R}_{\mathrm{cgs}}$ were known[3]. Our concern here, however, is the quantum non-zero temperature case, in which the restriction of paths to periodic functions is natural since the quantum partition function, which contains the thermodynamic information, involves making the trace of the kernel, and therefore restriction to periodic imaginary-time paths by definition.

Rescaling time $t \to t/T$ and defining $\Omega = 2\pi/T$ the bond action can be rewritten as

$$s\left(x, x'; \frac{2\pi}{\Omega}\right) = \frac{2\pi}{\Omega}\int_0^1 \left\{\frac{\Omega^2}{8\pi^2}\dot{x}^2 - \mathrm{v}\left(x, x'\right)\right\} dt, \tag{4}$$

and now $s$ acts on the space of period-one functions $x, x' : \mathbb{R}/\mathbb{Z} \to \mathbb{R}$ or *loops*.

Now let $\mathrm{x} \in \mathbb{R}^{\mathbb{Z}}$ be a classical ground state and call a bond action $s$ a $\tau$ or an $\upsilon$ as for the renormalization for classical ground states in [19]. For the case of mean spacing $\gamma^{-1}$ the sequence of bond actions then forms an infinite Fibonacci sequence of $\tau$ and $\upsilon$ types of bonds where each $\upsilon$ is always surrounded by $\tau$s. At this point one wants to eliminate all particles $z$ from sequences of the form $\upsilon(x, z; \Omega) + \tau(z, x'; \Omega)$ (for simplicity we use $\Omega$ as an argument of action bonds instead of $2\pi/\Omega$ from now on). In order to do this

[3]For example, we could obtain the scaling laws for the two particle correlation function $\langle x_n x_k \rangle$ if the eigenvalue of renormalization in the direction $\lambda\, x_n x_k$ was known.)

define the following decimation operator $\oplus$ acting on pairs of bond actions $(\upsilon, \tau)$ as

$$(\upsilon \oplus \tau)\left(x, x'; \Omega\right) = -\mathrm{i}\hbar \ln \int \mathcal{D}' z \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\left[\upsilon(x,z;\Omega)+\tau\left(z,x';\Omega\right)\right]}, \qquad (5)$$

such that $\exp\left[\frac{\mathrm{i}}{\hbar}\left(\upsilon \oplus \tau\right)(x, x'; \Omega)\right]$ is the traced kernel for particle $z$ as a function of its neighbours $x$ and $x'$. The decimated functional $\upsilon \oplus \tau$ still has the form of an action bond in the sense that it acts on pairs of loops $(x, x')$, and represents the effective coupling between $x$ and $x'$, the new bond action, still unscaled, once $z$ is integrated. The renormalization operator is defined as the composition of a decimation and scalings as

$$\mathcal{R}\left[\begin{array}{c} \tau\left(x, x'; \Omega\right) \\ \upsilon\left(x, x'; \Omega\right) \end{array}\right] = \frac{\mathcal{J}}{\varepsilon}\left[\begin{array}{c} \left(\upsilon \oplus \tau\right)\left(x/\alpha, x'/\alpha; \Omega/\varepsilon\right) \\ \tau\left(x/\alpha, x'/\alpha; \Omega/\varepsilon\right) \end{array}\right], \qquad (6)$$

which includes a scaling of frequencies, $\varepsilon$, still undetermined at this point. The global scaling of bond actions is $\mathcal{J}/\varepsilon$ instead of just $\mathcal{J}$ because the renormalization now acts on actions instead of energies as in the classical ground state case.

¿From equation (6) we see that the effect of renormalization acting on action bonds is to eliminate a subsequence of particles through decimation (5), resulting in an equivalent system where the undecimated particles are now coupled by renormalized action bonds. By performing the composition of (6) and (5) explicitly the natural scale factor $\kappa = \mathcal{J}/\varepsilon$ for Planck's constant arises, and $\mathcal{R}$ can be seen as acting on the extended space of $(\tau, \upsilon, \hbar)$ for $\hbar \geq 0$ as

$$\mathcal{R} : \left\{\begin{array}{l} \tilde{\tau}\left(x, x'; \Omega\right) = -\mathrm{i}\kappa\hbar \int \mathcal{D}' z \, \mathrm{e}^{\frac{\mathrm{i}}{\kappa\hbar}\frac{\mathcal{J}}{\varepsilon}\left\{\upsilon(x/\alpha,z;\Omega/\varepsilon)+\tau\left(z,x'/\alpha;\Omega/\varepsilon\right)\right\}} \\ \tilde{\upsilon}\left(x, x'; \Omega\right) = \frac{\mathcal{J}}{\varepsilon}\tau\left(x/\alpha, x'/\alpha; \Omega/\varepsilon\right) \\ \tilde{\hbar} = \kappa\hbar \end{array}\right. . \qquad (7)$$

We interpret $\kappa$ as the eigenvalue of $\mathcal{R}$ in the direction of Planck's constant.

Having constructed the renormalization operator we now want to find what can this tell us about the physical properties of FK models when we allow for non-zero $\hbar$. The complete picture of how $\mathcal{R}$ acts on the full parameter space (the renormalization *cascade*) is however typically difficult, if not impossible, to obtain. Fortunately, an analysis of the fixed points of $\mathcal{R}$ gives us some hints on the behaviour of the $\mathcal{R}$ cascade. E.g. distinct simple fixed points (with only attracting directions) and their basins of attraction corresponding to distinct phases in parameter space, and a critical fixed point (with both stable and unstable directions) with their stable manifolds are usually associated to boundaries between the distinct types of behaviour for the model. In the following subsection 2.1 we will show that, in the limit $\Omega, \hbar \to 0$, this choice of renormalization operator allows us to

recover the the classical ground state renormalization of [19] (this is shown in figure 2 - $\Omega$ direction not shown). As was mentioned in the introduction, this leads us to conclude that the renormalization (7) we introduce has a critical fixed point in the $\Omega, \hbar = 0$ subspace, which corresponds to the TBA. It is therefore a classical ground state fixed point, the boundary between a sliding or conducting region (subcritical) and a pinned or insulation one (supercritical). In order to consider how quantum effects change the behaviour of GFK models, we take into account in 2.2 the periodic motions of small $\Omega$, close to the classical TBA limit at $\Omega = 0$, and this allows us to determine the eigenvalue $\kappa$ in the quantum direction.

## 2.1 Semiclassical approximation and ground state limit

As a first step to connect the quantum renormalization (6) with the ground state renormalization of [19], one can look at the decimation operator (5) in the stationary phase approximation for small $\hbar$:

$$(\upsilon \oplus \tau)\left(x, x'; \Omega\right) = -\mathrm{i}\hbar \ln \int \mathcal{D}' z\, \delta\left(z - z_{\mathrm{cl.}}\left(x, x'; \Omega\right)\right) \times \\ \times \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\left\{\upsilon(x,z;\Omega)+\tau\left(z,x';\Omega\right)\right\}}. \tag{8}$$

Here $z_{\mathrm{cl.}}\left(x, x'; \Omega\right)$ is the classical path of period one satisfying the Euler–Lagrange equations

$$\left.\frac{\delta\left[\upsilon\left(x, z; \Omega\right) + \tau\left(z, x'; \Omega\right)\right]}{\delta z}\right|_{z = z_{\mathrm{cl.}}(x, x'; \Omega)} = 0. \tag{9}$$

In the classical limit one is thus left with a dynamical problem (9) and the decimated action (8) can be rewritten as

$$\underset{z \in \mathrm{loops}}{\mathrm{sta}} \left[\upsilon\left(x, z; \Omega\right) + \tau\left(z, x'; \Omega\right)\right], \tag{10}$$

the sum of bond actions evaluated at $z = z_{\mathrm{cl.}}$, given by (9), which stationarises the sum $\upsilon + \tau$ over the space of all loops $\{z : \mathbb{R}/\mathbb{Z} \to \mathbb{R}\}$.

### 2.1.1 Ground state limit

The ground state decimation can now be taken as the limit $\Omega \to 0$ of (8) or (10). To see this, notice that in this limit only the classical ground states contribute to the kernel and

$$\int \mathcal{D}' z\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\left\{\upsilon(x,z)+\tau\left(z,x'\right)\right\}} \simeq \mathrm{e}^{-\frac{2\pi \mathrm{i}}{\hbar\Omega}\left\{\mathrm{v}^{(\upsilon)}(\mathrm{x},\mathrm{z})+\mathrm{v}^{(\tau)}\left(\mathrm{z},\mathrm{x}'\right)\right\}},$$

where $(\mathrm{x}, \mathrm{z}, \mathrm{x}')$ is a segment of a classical ground state and $\mathrm{z}\left(\mathrm{x}, \mathrm{x}'\right)$ minimises the sum $\upsilon + \tau$. Taking the logarithm and multiplying by

$-\mathrm{i}\hbar$, this results in the decimation (5) being

$$\lim_{\Omega\to 0}\left[-\frac{\Omega}{2\pi}\left(\upsilon\oplus\tau\right)\left(x,x';\Omega\right)\right]=\min_{\mathrm{z}\in\mathbb{R}}\left[\mathrm{v}^{(\upsilon)}\left(\mathrm{x},\mathrm{z}\right)+\mathrm{v}^{(\tau)}\left(\mathrm{z},\mathrm{x}'\right)\right] \quad (11)$$

Apart from the limit factor $\lim_{\Omega\to 0}-2\pi/\Omega$ this is in fact the classical ground state decimation in [19] and so the renormalization (6) becomes[4]

$$\begin{aligned}\mathcal{R}\left[\begin{array}{c}\tau\left(x,x';0\right)\\ \upsilon\left(x,x';0\right)\end{array}\right] &\simeq \lim_{\Omega\to 0}\left[\begin{array}{c}-\frac{2\pi}{\Omega}\mathcal{J}\left(\mathrm{v}^{(\upsilon)}\oplus_{\mathrm{cgs}}\mathrm{v}^{(\tau)}\right)\left(\mathrm{x}/\alpha,\mathrm{x}'/\alpha\right)\\ -\frac{2\pi}{\Omega}\mathcal{J}\mathrm{v}^{(\tau)}\left(\mathrm{x}/\alpha,\mathrm{x}'/\alpha\right)\end{array}\right]\\ &= \lim_{\Omega\to 0}-\frac{2\pi}{\Omega}\mathcal{R}_{\mathrm{cgs}}\left[\begin{array}{c}\mathrm{v}^{(\tau)}\left(\mathrm{x},\mathrm{x}'\right)\\ \mathrm{v}^{(\upsilon)}\left(\mathrm{x},\mathrm{x}'\right)\end{array}\right], \quad (12)\end{aligned}$$

where $\oplus_{\mathrm{cgs}}$ and $\mathcal{R}_{\mathrm{cgs}}$ are the decimation and renormalization operators for the classical ground states, and $\varepsilon\in\mathbb{R}$ is still undetermined. The renormalization $\mathcal{R}$ has therefore a fixed point (the TBA fixed point), with ground states of mean spacing $\rho=\gamma^{-1}$, in the $\Omega=0$ subspace consisting of

$$\left[\begin{array}{c}\bar{\tau}\left(x,x';0\right)\\ \bar{\upsilon}\left(x,x';0\right)\end{array}\right]=\lim_{\Omega\to 0}-\frac{2\pi}{\Omega}\left[\begin{array}{c}\bar{\mathrm{v}}^{(\tau)}\left(x,x'\right)\\ \bar{\mathrm{v}}^{(\upsilon)}\left(x,x'\right)\end{array}\right],$$

where $(\bar{\mathrm{v}}^{\tau},\bar{\mathrm{v}}^{\upsilon})$ is the fixed point of the ground state renormalization operator $\mathcal{R}_{\mathrm{cgs}}$, because applying expression (12) at the TBA fixed point results in

$$\mathcal{R}\left[\begin{array}{c}\bar{\tau}\left(x,x';0\right)\\ \bar{\upsilon}\left(x,x';0\right)\end{array}\right]=\lim_{\Omega\to 0}-\frac{2\pi}{\Omega}\left[\begin{array}{c}\bar{\mathrm{v}}^{(\tau)}\left(\mathrm{x},\mathrm{x}'\right)\\ \bar{\mathrm{v}}^{(\upsilon)}\left(\mathrm{x},\mathrm{x}'\right)\end{array}\right]=\left[\begin{array}{c}\bar{\tau}\left(x,x';0\right)\\ \bar{\upsilon}\left(x,x';0\right)\end{array}\right].$$

We have thus shown that renormalization (6) behaves in the manner we intended, namely that we recover the classical ground state renormalization[5] and that the critical TBA point is still a (necessarily critical) fixed point of the quantum renormalization $\mathcal{R}$ in the classical, zero frequency subspace.

## 2.2 Renormalization for the phonon spectrum

Close to the ground state, for small $\Omega^2$, the relevant contributions are approximately given by the normal modes or *phonons*. For a GFK model at irrational mean spacing ground state, $\rho$, the phonon spectrum includes zero in the subcritical regime, but the minimum

[4] We take the formal equality $f\left(\Omega=0\right)=\lim_{\Omega\to 0}g\left(\Omega\right)$ with the meaning $\lim_{\Omega\to 0}\left[f\left(\Omega\right)/g\left(\Omega\right)\right]=1$, even if both quantities $f\left(\Omega\right)$ and $g\left(\Omega\right)$ diverge in this limit.

[5] We recall that the factor $-2\pi/\Omega$ is due to the fact that we now renormalize bond actions instead of bond energies, and so has a dimensional origin. Note that we could have formulated renormalization on quantities with dimensions of energy, namely $-\Omega/2\pi\times$(action bonds) in equation (4), thus avoiding the $-2\pi/\Omega$ factor in equation (12).

frequency or *phonon gap* is positive above the critical point $u_c$ [5]. The phonon contribution to the trace of the kernel is given by doing a quadratic approximation which is (with $x_n = \mathrm{x}_n + \xi_n$)

$$K'\left(\mathrm{x}, \frac{2\pi}{\Omega}\right) \simeq \mathrm{e}^{-\frac{2\pi \mathrm{i}}{\hbar\Omega}\sum_n \mathrm{v}^{(n)}\left(\mathrm{x}_n, \mathrm{x}_{n+1}\right)} \times \tag{13}$$
$$\times \int \mathcal{D}'\xi\, \mathrm{e}^{\frac{\pi \mathrm{i}}{\hbar\Omega}\sum_n \int_0^1 \left\{\frac{\Omega^2}{4\pi^2} m^{(n)}\left(\dot\xi_n, \dot\xi_{n+1}\right) - u^{(n)}\left(\xi_n, \xi_{n+1}\right)\right\} dt},$$

where the kinetic term was generalised to a symmetric quadratic form in the velocities

$$m^{(n)}\left(\dot\xi, \dot\xi'\right) = m_{11}^{(n)}\dot\xi^2 + 2m_{12}^{(n)}\dot\xi\,\dot\xi' + m_{22}^{(n)}\,\dot\xi'^{\,2}$$

(as will become clear later on the renormalization operator introduces coupling between the velocities of neighbouring particles), and $u$ is also a symmetric quadratic form

$$u^{(n)}\left(\xi, \xi'\right) = u_{22}^{(n)}\xi^2 - 2u_{12}^{(n)}\xi\xi' + u_{11}^{(n)}\xi'^2.$$

The first term in (13) is simply the classical ground state and corresponds to (12), so one wants to apply the decimation (5) to the sum of the quadratic parts of bond actions of the form

$$\frac{\pi}{\Omega}\left\{\frac{\Omega^2}{4\pi^2}\left[m^{(\upsilon)}\left(\dot\xi, \dot\zeta\right) + m^{(\tau)}\left(\dot\zeta, \dot\xi'\right)\right] - \left[u^{(\upsilon)}\left(\xi, \zeta\right) + u^{(\tau)}\left(\zeta, \xi'\right)\right]\right\}.$$

Because this sum is quadratic in the particle to eliminate, $\zeta$, the corresponding functional integral can be calculated (for example by Gaussian integration of the Fourier transformed sum of action bonds [28]) and the semiclassical approximation is exact in this case. To first order in $\Omega^2$ the result is[6]

$$\mathrm{e}^{\frac{\mathrm{i}\pi}{\hbar\Omega}\left\{\frac{\Omega^2}{4\pi^2}\left[m^{(\upsilon)}\left(\dot\xi, \dot\zeta\right) + m^{(\tau)}\left(\dot\zeta, \dot\xi'\right)\right] - \left[u^{(\upsilon)}\left(\xi, \zeta\right) + u^{(\tau)}\left(\zeta, \xi'\right)\right]\right\}} \simeq$$
$$\simeq \mathrm{e}^{\frac{\mathrm{i}\pi}{\hbar\Omega}\left\{\frac{\Omega^2}{4\pi^2}\tilde m^{(\tau)}\left(\dot\xi, \dot\xi'\right) - \tilde u^{(\tau)}\left(\xi, \xi'\right)\right\}},$$

where $\tilde m^{(\tau)}$ is a new symmetric quadratic form with components

[6] There is possibly also a logarithmic term due to the integration measure which corresponds to a redefinition of the ground state energy.

given by

$$\begin{aligned}
\tilde{m}_{11}^{(\tau)} &= m_{11}^{(\upsilon)} + \frac{2m_{12}^{(\upsilon)}u_{12}^{(\upsilon)}}{u_{22}^{(\upsilon)}+u_{11}^{(\tau)}} + \frac{\left(m_{22}^{(\upsilon)}+m_{11}^{(\tau)}\right)u_{12}^{(\upsilon)2}}{\left(u_{22}^{(\upsilon)}+u_{11}^{(\tau)}\right)^2} \\
\tilde{m}_{12}^{(\tau)} &= \frac{m_{12}^{(\upsilon)}u_{12}^{(\tau)}+m_{12}^{(\tau)}u_{12}^{(\upsilon)}}{u_{22}^{(\upsilon)}+u_{11}^{(\tau)}} + \frac{\left(m_{22}^{(\upsilon)}+m_{11}^{(\tau)}\right)u_{12}^{(\upsilon)}u_{12}^{(\tau)}}{\left(u_{22}^{(\upsilon)}+u_{11}^{(\tau)}\right)^2} \qquad (14) \\
\tilde{m}_{22}^{(\tau)} &= m_{22}^{(\tau)} + \frac{2m_{12}^{(\tau)}u_{12}^{(\tau)}}{u_{22}^{(\upsilon)}+u_{11}^{(\tau)}} + \frac{\left(m_{22}^{(\upsilon)}+m_{11}^{(\tau)}\right)u_{12}^{(\tau)2}}{\left(u_{22}^{(\upsilon)}+u_{11}^{(\tau)}\right)^2}
\end{aligned}$$

and the new form $\tilde{u}^{(\tau)}$ has components

$$\begin{aligned}
\tilde{u}_{11}^{(\tau)} &= u_{11}^{(\upsilon)} - \frac{u_{12}^{(\upsilon)2}}{u_{22}^{(\upsilon)}+u_{11}^{(\tau)}} \\
\tilde{u}_{12}^{(\tau)} &= \frac{u_{12}^{(\upsilon)}u_{12}^{(\tau)}}{u_{22}^{(\upsilon)}+u_{11}^{(\tau)}} \qquad (15) \\
\tilde{u}_{22}^{(\tau)} &= u_{22}^{(\tau)} - \frac{u_{12}^{(\tau)2}}{u_{22}^{(\upsilon)}+u_{11}^{(\tau)}}.
\end{aligned}$$

With these new quadratic forms, the decimation (5) becomes simply

$$\begin{aligned}
(\upsilon \oplus \tau)\left(x,x';\Omega\right) &= (\text{c.g.s. decimation}) + \qquad (16) \\
&+ \frac{1}{\Omega}\int_0^1 \Omega^2 \tilde{m}^{(\tau)}\left(\xi,\xi'\right) - \tilde{u}^{(\tau)}\left(\xi,\xi'\right)\, dt,
\end{aligned}$$

where 'c.g.s decimation' is the decimation (11). For the renormalization (6) one also needs the 'undecimated' bond actions which correspond to isolated bond actions of type $\tau$, so one should define also

$$\begin{aligned}
\tilde{m}^{(\upsilon)}\left(\xi,\xi'\right) &= m^{(\tau)}\left(\xi,\xi'\right) \\
\tilde{u}^{(\upsilon)}\left(\xi,\xi'\right) &= u^{(\tau)}\left(\xi,\xi'\right).
\end{aligned} \qquad (17)$$

For a GFK model (3) at the start of renormalization, for either type $\tau$ or $\upsilon$ of bonds the quadratic forms are $m_{12}=0$, $m_{11}+m_{22}=1$, $u_{jj} = \mathrm{v}_{,jj}\left(\mathrm{x},\mathrm{x}'\right)$ for $j=1,2$ and $u_{12} = -\mathrm{v}_{,12}\left(\mathrm{x},\mathrm{x}'\right)$, where the subscripts in v denote differentiation with respect to the first and second variables and $(\mathrm{x},\mathrm{x}')$ is a segment of a classical ground state. Because $u$ is then dependent on $(\mathrm{x},\mathrm{x}')$, after iterating the above transformations (14), (15) and (17) one ends up with a set of asymptotic quadratic forms depending on the ground state, $\bar{m}_{\mathrm{x},\mathrm{x}'}^{(\tau)}$, $\bar{m}_{\mathrm{x},\mathrm{x}'}^{(\upsilon)}$, $\bar{u}_{\mathrm{x},\mathrm{x}'}^{(\tau)}$ and $\bar{u}_{\mathrm{x},\mathrm{x}'}^{(\upsilon)}$ which

scale by factors[7] $\omega = \alpha^2\varepsilon^2/\mathcal{J} \simeq 1.255\,071$ for the mass forms and $\mathcal{J}/\alpha^2$ for the potential forms [19], i.e.

$$\left\{\begin{array}{l} \tilde{\bar{m}}^{(\tau)}_{\mathrm{x},\mathrm{x}'} \simeq \frac{\alpha^2\varepsilon^2}{\mathcal{J}}\bar{m}^{(\tau)}_{\mathrm{x},\mathrm{x}'} \\ \tilde{\bar{m}}^{(\upsilon)}_{\mathrm{x},\mathrm{x}'} \simeq \frac{\alpha^2\varepsilon^2}{\mathcal{J}}\bar{m}^{(\tau)}_{\mathrm{x},\mathrm{x}'} \\ \tilde{\bar{u}}^{(\tau)}_{\mathrm{x},\mathrm{x}'} \simeq \frac{\alpha^2}{\mathcal{J}}\bar{u}^{(\tau)}_{\mathrm{x},\mathrm{x}'} \\ \tilde{\bar{u}}^{(\upsilon)}_{\mathrm{x},\mathrm{x}'} \simeq \frac{\alpha^2}{\mathcal{J}}\bar{u}^{(\upsilon)}_{\mathrm{x},\mathrm{x}'} \end{array}\right. . \tag{18}$$

Finally, using (14–18), and defining

$$\begin{aligned} \bar{\tau}\left(x,x';\Omega\right) &:= \frac{\pi}{\Omega}\left[-\bar{\mathrm{v}}^{(\tau)}\left(\mathrm{x},\mathrm{x}'\right)\right. \\ &+ \left.\int_0^1\left\{\frac{\Omega^2}{4\pi^2}\bar{m}^{(\tau)}_{\mathrm{x},\mathrm{x}'}\left(\xi,\xi'\right) - \bar{u}^{(\tau)}_{\mathrm{x},\mathrm{x}'}\left(\xi,\xi'\right)\right\}dt\right] \\ \bar{\upsilon}\left(x,x';\Omega\right) &:= \frac{\pi}{\Omega}\left[-\bar{\mathrm{v}}^{(\upsilon)}\left(\mathrm{x},\mathrm{x}'\right)\right. \\ &+ \left.\int_0^1\left\{\frac{\Omega^2}{4\pi^2}\bar{m}^{(\tau)}_{\mathrm{x},\mathrm{x}'}\left(\xi,\xi'\right) - \bar{u}^{(\tau)}_{\mathrm{x},\mathrm{x}'}\left(\xi,\xi'\right)\right\}dt\right], \end{aligned}$$

the renormalization (7) at $(\bar{\tau},\bar{\upsilon},\hbar)$ becomes

$$\mathcal{R}\left[\begin{array}{c} \bar{\tau}\left(x,x';\Omega\right) \\ \bar{\upsilon}\left(x,x';\Omega\right) \\ \hbar \end{array}\right] \simeq \left[\begin{array}{c} \bar{\tau}\left(x,x';\Omega\right) \\ \bar{\upsilon}\left(x,x';\Omega\right) \\ \kappa\hbar \end{array}\right].$$

Thus, by including the scaling of frequencies $\varepsilon \simeq 1.649\,415$ (see footnote 7) in the renormalization (6), the point $(\bar{\tau},\bar{\upsilon},0)$ becomes an approximate fixed point for small $\Omega$ (actually a line of fixed points parametrised by $\Omega$). In particular the phonon spectrum is asymptotically self-similar under scaling by $\varepsilon$ in the direction of $\Omega$.

Finally, note that fixing $\varepsilon$ also determines the eigenvalue in the $\hbar$-direction[8] as $\kappa = \mathcal{J}/\varepsilon \simeq 2.630\,716$.

## 2.3 Scaling of the kernel

The results in subsection 2.2 imply that the effect of including both the frequencies and quantum directions, close to the TBA fixed point (for $\Delta u := u - u_c$, $\Delta P := P - P_{\gamma^{-1}}(u_c)$, $\Omega$ and $\hbar$ small), is that the

[7] In [19] the scaling is actually for the quantities $a_n := u_{22}^{(n-1)} + u_{11}^{(n)}$, $b_n := u_{12}^{(n)}$, $c_n := m_{22}^{(n-1)} + m_{11}^{(n)}$ and $d_n := m_{12}^{(n)}$ with scaling constants $\omega \simeq 1.255\,071$ for $a_n$ and $b_n$ and $\beta/\alpha$ for $c_n$ and $d_n$, so the first and third equations in (18) are defined up to a quadratic coboundary. Here we use the scale factors for frequency $\varepsilon := \sqrt{\omega\mathcal{J}/\alpha^2} \simeq 1.649\,415$ and energy $\mathcal{J} = \alpha\beta$ instead. The origin of $\omega$ is still a mystery.

[8] This result was published in [12] containing a mistake: $k = \mathcal{J}\varepsilon$ instead of the correct value $\kappa = \mathcal{J}/\varepsilon$.

following asymptotic relation of bond actions (regarded as functions in parameter space) holds

$$(\tau, \upsilon)\,(\Delta u, \Delta P, \Omega, \hbar) \simeq \frac{\mathcal{J}}{\varepsilon}\,(\tau, \upsilon)\,(\delta\Delta u, \eta\Delta P, \varepsilon\Omega, \kappa\hbar)\,. \tag{19}$$

If $K'_{J,F_m}$ is the trace of the kernel for a chain of size $F_m$, the $m$th Fibonacci number, in the discretised form with $J$ 'time steps' (such that $K'_{F_m} = \lim_{J\to\infty} K'_{J,F_m}$), then

$$K'_{J,F_m}\,(\Delta u, \Delta P, \Omega, \hbar) \simeq K'_{J,F_{m-1}}\,(\delta\,\Delta u, \eta\,\Delta P, \varepsilon\,\Omega, \kappa\,\hbar)\left(\frac{\sqrt{\mathcal{J}}}{|\alpha|\,\varepsilon}\right)^{JF_{m-1}}. \tag{20}$$

Here the multiplying factor comes from the functional integration measure due to the change of coordinates (here with diagonal mass components $\mu^{(n)} = \bar{m}_{22}^{(n-1)} + \bar{m}_{11}^{(n)}$)

$$\begin{aligned}\prod_n \left(\mathcal{D}'_J \frac{x_n}{\alpha}\right)(\Omega, \hbar) &= \prod_n \prod_{j=0}^{J-1} \sqrt{\frac{\mu^{(n)}\Omega J}{4\pi^2 \mathrm{i}\,\hbar}}\,\frac{dx_n^{(j)}}{|\alpha|} \\ &= \prod_n \left(\frac{\sqrt{\mathcal{J}}}{|\alpha|\,\varepsilon}\right)^J \left(\mathcal{D}'_J \tilde{x}_n\right)(\varepsilon\Omega, \kappa\hbar)\,,\end{aligned}$$

where $\tilde{x}_n$ are the positions of the renormalized particles.

We stress that the scaling relation (20) is asymptotically exact as we approach the TBA (classical) point. In our analysis of renormalization the phonon contribution leading to (20), we have made use of the stationary phase approximation, which does not take into account interactions between degenerate minima (i.e. tunnelling effects), even though the renormalization (7) does. Yet, equation (20) is asymptotically exact in the limit $\hbar \to 0$ subspace, where tunnelling contributions do not play a role. Tunnelling is instead important when $\hbar$ is large, and the numerical results of [27] show that for $\hbar > 0$ there is a transition at $u > u_c$ (this is illustrated in figure 3).

Figure 3: Proposed splitting of the $u - \hbar$ space into a phonon region and a Bloch region. The black area represents transitional behaviour, where Bloch spectral bands merge into a unique phonon band, motivated by our renormalization approach which suggest a transition curve originating from the TBA point ($\hbar = 0$) and the results of [27] showing that a transition region exists for some $\hbar > 0$ when $u > u_c\,(\hbar = 0)$.

As we mention in the introduction, our aim is to study non-zero temperature or statistical mechanics problem, in particular to obtain scaling laws for thermodynamic quantities. Having obtained the scaling equation (20) for the kernel, it is straightforward to obtain an equivalent relation for the partition function $\mathcal{Z}$ by 'Wick rotation', which we proceed to do in the next section.

## 2.4 Non-zero temperature scaling

The quantum partition function at temperature $\Theta$ can be easily obtained from the trace of the kernel by Wick rotation, i.e. doing $2\pi/\Omega = -\mathrm{i}\beta\hbar$, where $\beta = 1/\Theta$. The quantum partition function is then

$$\mathcal{Z}(\beta\hbar, \hbar) = K'(-\mathrm{i}\beta\hbar, \hbar) = \int \mathcal{D}'x \, \mathrm{e}^{-\beta \mathcal{S}_E(x;\beta\hbar)}, \tag{21}$$

where the *Euclidean action* for the FK model is

$$\begin{aligned} \mathcal{S}_E &= \sum_n s_E(x_n, x_{n+1}; \beta\hbar) \\ &= \sum_n \int_0^1 \left\{ \frac{\dot{x}_n^2}{2(\beta\hbar)^2} + \mathrm{v}(x_n, x_{n+1}) \right\} dt_E, \end{aligned}$$

and the integration is now over the rescaled Euclidean time $t_E \in \mathbb{R}/\mathbb{Z}$. Comparing with (4), the *Euclidean bond action* $s_E$ can be written as

$$s_E(x, x'; \beta\hbar) = \left[ -\frac{\Omega}{2\pi} s(x, x'; \Omega) \right]_{\Omega = 2\pi\mathrm{i}/\beta\hbar},$$

and has units of an energy instead of an action because of the multiplying factor $\Omega/2\pi$. This gives another direction to which renormalization can be extended, the temperature direction $\Theta = 1/\beta$. Define then the operator $\oplus_E$ by 'Wick rotating' the operator $\oplus$ for the trace of the kernel (5), to obtain

$$(\upsilon_E \oplus_E \tau_E)(x, x'; \beta\hbar) = -\beta^{-1} \ln \int \mathcal{D}'z \, \mathrm{e}^{-\beta\left[\upsilon_E(x,z;\beta\hbar) + \tau_E(z,x';\beta\hbar)\right]},$$

and the renormalization as

$$\mathcal{R}_E \begin{bmatrix} \tau_E(x, x'; \beta\hbar) \\ \upsilon_E(x, x'; \beta\hbar) \end{bmatrix} = \begin{bmatrix} \mathcal{J}(\upsilon_E \oplus_E \tau_E)(x/\alpha, x'/\alpha; \varepsilon\beta\hbar) \\ \mathcal{J}\tau_E(x/\alpha, x'/\alpha; \varepsilon\beta\hbar) \end{bmatrix}. \tag{22}$$

Therefore, close to the TBA fixed point the renormalization operator leads to the corresponding relation to (19) for Euclidean bond actions:

$$(\tau_E, \upsilon_E)(\Delta u, \Delta P, \beta\hbar, \hbar) \simeq \mathcal{J}(\tau_E, \upsilon_E)\left(\delta\Delta u, \eta\Delta P, \varepsilon^{-1}\beta\hbar, \kappa\hbar\right), \tag{23}$$

so under the renormalization $\mathcal{R}_E$ there is a fixed point at $\hbar = 0$, $\beta\hbar = \infty$, with an unstable eigenvalue of $\kappa\varepsilon = \mathcal{J} \simeq 4.339\,143\,9$ in the temperature direction.

Although this agrees with the scaling of [21] for classical statistical mechanics, the result here includes the momentum contribution and corresponds to the quantum correction of the low temperature classical result, in the region $\Theta \ll \hbar$ in which the classical partition function is not valid (see [11, section 3.2]). In fact, we think that the

classical results in [21] are an indication of the existence of another fixed point of our quantum renormalization operator (22), namely a fixed point for $\beta\hbar = 0$. This should require that the kinetic part of the classical partition function is also renormalized (we recall that in [21] the renormalization acts exclusively on the potential contributions) in order to be able to extend the analysis to non-zero Planck's constant. The existence of a $\beta\hbar = 0$ fixed point is however independent of our present analysis, and requires further investigation.

Denoting by $\mathcal{Z}_{F_m}(\Delta u, \Delta P, \Theta, \hbar)$ the quantum partition function for a chain of $F_m$ particles at temperature $\Theta$, regarded as a function in parameter space, the renormalization picture leads to

$$\mathcal{Z}_{F_m}(\Delta u, \Delta P, \Theta, \hbar) \simeq \mathcal{Z}_{F_{m-1}}(\delta\,\Delta u, \eta\,\Delta P, \mathcal{J}\,\Theta, \kappa\,\hbar)\left(\frac{\sqrt{\mathcal{J}}}{|\alpha|\,\varepsilon}\right)^{JF_{m-1}}. \tag{24}$$

The free energy $f = -\Theta \lim_{m\to\infty} \ln \mathcal{Z}_{F_m}/F_m$ therefore behaves like

Figure 4: Example of the behaviour of $c_P$ for the choice of $k(a,b) = [c^+k^+(a,b) + c^-k^-(a,b)]\,\mathrm{e}^{-c\left(\frac{a}{\ln\mathcal{J}} - \frac{b}{\ln\kappa}\right)}$ in equation (27) with $c = 1/2$, $c^+ = 1$, $c^- = 1/5$ and $k^\pm = 1 + \cos 2\pi\left(\frac{a}{\ln\mathcal{J}} \pm \frac{b}{\ln\kappa}\right)$. Lighter shading corresponds to larger values of $c_P(\Theta, \hbar)$.

(using $\gamma^{-1} = \lim_{m\to\infty} F_{m-1}/F_m$)

$$f(\Delta u, \Delta P, \Theta, \hbar) \simeq \frac{1}{\gamma\mathcal{J}} f(\delta\,\Delta u, \eta\,\Delta P, \mathcal{J}\,\Theta, \kappa\,\hbar) - \frac{\Theta J}{\gamma}\ln\left(\frac{\sqrt{\mathcal{J}}}{|\alpha|\,\varepsilon}\right), \tag{25}$$

close to the TBA fixed point, and $e = -\Theta^2\,\partial(f/\Theta)/\partial\Theta$, the energy per particle, like

$$e(\Delta u, \Delta P, \Theta, \hbar) \simeq \frac{1}{\gamma\mathcal{J}} e(\delta\,\Delta u, \eta\,\Delta P, \mathcal{J}\,\Theta, \kappa\,\hbar).$$

This leads to the following scaling law for the specific heat per particle at constant pressure $c_P = \partial e/\partial\Theta$:

$$c_P(\Delta u, \Delta P, \Theta, \hbar) \simeq \gamma^{-1} c_P(\delta\,\Delta u, \eta\,\Delta P, \mathcal{J}\,\Theta, \kappa\,\hbar). \tag{26}$$

We note that because we construct a *discrete* renormalization procedure, the solutions of our scaling equations allow not only power law behaviour, but also other types of self-similar behaviour. In particular, close to the TBA, with $\Delta u = \Delta P = 0$ for small $\Theta$ and $\hbar$, equation (26) allows for solutions of the form

$$c_P(\Theta, \hbar) \simeq \Theta^{\frac{\ln\gamma}{\ln\mathcal{J}}}\, k(\ln\Theta, \ln\hbar), \tag{27}$$

with $k(a + \ln\mathcal{J}, b + \ln\kappa) = k(a,b)$, for all $a$ and $b$. Taking into account the findings of [25, 24, 26], which show a hierarchical behaviour

of thermodynamic quantities in the classical case, e.g. through a sequence of increasing jumps (*Schottky anomalies*) in the specific heat, as temperature is increased - the *hierarchical melting* of the chain - , our renormalization picture suggests that close to the TBA this behaviour can be extended to the $(\Theta, \hbar)$-plane through a the sequence of modulated ridges, invariant under scaling by $(\mathcal{J}, \kappa)$, of which we show an example in figure 4.

# 3 Summary and conclusions

In summary, we propose a generalisation of the classical Transition by Breaking of Analyticity by extending the renormalization to non-zero Planck's constant and temperature, $\Theta$. We construct a renormalization operator adapted to quantum thermodynamics by partial integration of the partition function, and deduce scaling eigenvalues in the direction of both $\hbar$ and $\Theta$. We point as our main results both the scaling equations 23–26 and the technique we present of extending the study of a classical ground state critical point to quantum statistical mechanics by making use of a the scaling of the phonon spectrum.

Our analysis shows that there is a new unstable eigenvalue $\kappa$ of renormalization in the $\hbar$. In particular concerning the question of 'long–range order', the intuitive picture would be that the non-zero Planck's regime is attracted to some high $\hbar$, possibly infinite (i.e. free particle), limit, where long range order is absent. However, the characterisation of a the system by the analysis of renormalization fixed points is local, limited to a small region close to the fixed point, and one should be cautious when extrapolating the results to regions far from the fixed point. Another factor that can be of importance is that the behaviour of the system can be dominated by other eigenvalues larger than $\kappa$ of which we have no knowledge. To gain a complete picture of the behaviour of Frenkel–Kontorova models for the full parameter space (including temperature and Planck's constant) further investigation, both theoretical and numerical is thus needed.

# Acknowledgements

NRC was funded by the Portuguese institution 'Fundação para a Ciência e Tecnologia' under the reference PRAXIS XXI/BD/21987/99.

# References

[1] S. Aubry. The devil's stair case transformation in incommensurate lattices. In D. Chudnovsky and G. Chudnovsky, editors,

*The Riemann Problem, Complete Integrability and Arithmetic Solutions*, volume 925 of *Springer Lecture Notes in Mathematics*. Springer-Verlag, 1982.

[2] S. Aubry. Devil's staircase and order without periodicity in classical condensed matter. *Journal de Physique*, 44:147–162, 1983.

[3] S. Aubry. The twist map, the extended Frenkel–Kontorova model and the devil's staircase. *Physica D*, 7:240–258, 1983.

[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. *Physica D*, 8:381–422, 1983.

[6] G. P. Berman, E. N. Bulgakov, and D. K. Campbell. Coherent structures in the ground state of the quantum Frenkel–Kontorova model. *Physical Review B*, 49:8212–8226, 1994.

[7] G. P. Berman, E. N. Bulgakov, and D. K. Campbell. Rugged landscapes and the "Quantori" ground state of 1D quantum systems of adatoms on substrates. *Physica D*, 107:161–165, 1997.

[8] F. Borgonovi, I. Guarneri, and D. Shepelyansky. Quantum effects in the Frenkel–Kontorova model. *Physical Review Letters*, 63:2010–2012, 1989.

[9] F. Borgonovi, I. Guarneri, and D. Shepelyansky. Destruction of classical cantori in the the quantum Frenkel–Kontorova model. *Zeitschrift für Physik B*, 79:133–142, 1990.

[10] O. M. Braun and Y. S. Kivshar. *The Frenkel–Kontorova Model, Concepts, Methods, and Applications*. Springer-Verlag, 2004.

[11] N. R. Catarino. *Quantum Statistical Mechanics of Generalised Frenkel–Kontorova Models*. PhD thesis, Mathematics Institute, University of Warwick, 2004.

[12] N. R. Catarino and R. S. MacKay. Quantum statistical mechanics of Frenkel–Kontorova models. In L. Vázquez, R. S. MacKay, and M.-P. Zorzano, editors, *Localization and Energy Transfer in Nonlinear Systems*, pages 315–319. World-Scientific, 2003.

[13] R. Giachetti and V. Tognetti. Variational approach to quantum statistical mechanics of nonlinear systems with application to sine–Gordon. *Physical Review Letters*, 55:912–915, 1985.

[14] R. Giachetti and V. Tognetti. Quantum corrections to the thermodynamics of nonlinear systems. *Physical Review B*, 33:7647–7658, 1986.

[15] J. M. Greene. A method for determining a stochastic transition. *Journal of Mathematical Physics*, 20:1183–1201, 1979.

[16] C.-L. Ho and C.-I. Chou. Simple variational approach to the quantum Frenkel–Kontorova model. *Physical Review E*, 63:016203(5), 2000.

[17] B. Hu, B. Li, and W.-M. Zang. Quantum Frenkel–Kontorova model: A squeezed state approach. *Physical Review E*, 58:R4068–R4071, 1998.

[18] H. Koch. A renormalization group fixed point associated with the breakup of golden invariant tori. *Discrete and Continuous Dynamical Systems*, 11(4):881–909, 2004.

[19] R. S. MacKay. Scaling exponents at the transition by breaking of analyticity for incommensurate structures. *Physica D*, 50:71–79, 1991.

[20] R. S. MacKay. *Renormalisation in Area–Preserving Maps*, volume 6 of *Advanced Series in Nonlinear Dynamics*. World-Scientific, 1993.

[21] R. S. MacKay. The classical statistical mechanics of Frenkel–Kontorova models. *Journal of Statistical Physics*, 80:45–67, 1995.

[22] J. W. Negele and H. Orland. *Quantum Many-Particle Systems*. Perseus Books, 1998.

[23] M. Peyrard and S. Aubry. Critical behaviour at the transition by breaking of analyticity in the discrete Frenkel–Kontorova model. *Journal of Physics C*, 16:1593–1608, 1983.

[24] R. Schilling and S. Aubry. The static structure factor of one-dimensional non-analytic incommensurate structures. *Journal of Physics C*, 20:4881–4889, 1987.

[25] F. Vallet, R. Schilling, and S. Aubry. Hierarchical low-temperature behaviour of one-dimensional incommensurate structures. *Europhysics Letters*, 2:815–822, 1986.

[26] F. Vallet, R. Schilling, and S. Aubry. Low-temperature excitations, specific heat and hierarchical melting of a one-dimensional incommensurate structure. *Journal of Physics C*, 21:67–105, 1988.

[27] O. V. Zhirov, G. Casati, and D. L. Shepelyansky. Quantum phase transition in the Frenkel–Kontorova chain: From pinned instanton glass to sliding phonon gas. *Physical Review E*, 67:056209(14), 2003.

[28] J. Zinn-Justin. *Quantum Field Theory and Critical Phenomena*. Oxford University Press, 2002 [1989].