QUANTUM STATISTICAL MECHANICS OF FRENKEL–KONTOROVA MODELS

NUNO R CATARINO & ROBERT S MACKAY

Mathematics Institute, University of Warwick, Gibbet Hill Road, Coventry CV4 7AL, UK
E-mail: catarino@maths.warwick.ac.uk, E-mail: mackay@maths.warwick.ac.uk

We generalise the classical Transition by Breaking of Analyticity in the Frenkel–Kontorova model 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.

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 sine–Gordon) with Lagrangian

$$L[x] = \sum_{n\in \mathsf{Z}} \left\{ \frac{m\dot{x}_n^2}{2} - \mathsf{v}[x_n, x_{n+1}] \right\}, \tag{1}$$

where

$$\mathsf{v}[x, x'] = \frac{w}{2}(x'-x)^2 + p(x'-x) + \frac{u}{4\pi^2}\cos[2\pi x]. \tag{2}$$

Here, the period of the onsite potential has been scaled to one. The mass m and coupling constant w can also be scaled to one.

For $u = 0$ its *minimum energy configurations* (i.e. $x \in \mathsf{R}^{\mathsf{Z}}$ such that $\forall M < m < N, V_{M,N}(x) \equiv \sum_{n=M}^{N-1} \mathsf{v}(x_n, x_{n+1})$ is minimum for all variations of x_m) are arrays of equally spaced particles and the *mean spacing* ρ is simply $-p/w$. In the opposite limit, $w = 0$, all particles are in the minima of the onsite potential and the mean spacing is the closest integer to $-p/w$ (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 ρ there there is a curve $p = p_c(u)$ of mean spacing ρ containing one critical value u_c (for other potentials there may be more than one u_c). The regime for u less than u_c is called *subcritical* (or *sliding phase*) and above u_c *supercritical* (or *pinned phase*) [1].

We call successive pairs (x_n, x_{n+1}) *bonds* and $\mathsf{v}(x_n, x_{n+1})$ the *energy of the bond*. Considering in particular the case of mean spacing $\rho = \gamma^{-1}$ where $\gamma = \frac{1+\sqrt{5}}{2}$ is the golden mean, relabeling the bonds v appropriately [2] as τ and υ results in a Fibonacci sequence of τs and υs. The TBA point can be viewed as a fixed point of the renormalization operator that minimises the energy of the sum of successive υ and τ-bonds with suitably chosen space and energy scalings, $\alpha, J \in \mathsf{R}$ respectively (depending on (υ, τ)) (actually it is also necessary to subtract a constant and a quadratic coboundary but we will suppress reference to these inessential terms).

The renormalization operator has a nontrivial fixed point (υ^*, τ^*) with $\alpha \simeq -1.414\,836\,0$ and $J \simeq 4.399\,143\,9$. 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'll call the p direction), with eigenvalue $\eta = -J/\gamma \simeq -2.681\,738\,4$ [2].

2 Phonon Spectrum

The *phonon spectrum* of a configuration is the set of frequencies of the linearised vibrations about it. For the FK model with irrational ρ the phonon spectrum includes 0 in the subcritical regime, but the minimum phonon frequency becomes positive above the critical point [1] u_c.

The classical action for time-periodic solutions of the FK model (of period T) is

$$S(x;T) = \sum_{n\in \mathsf{Z}} s(x_n, x_{n+1}; T), \qquad s(x,x';T) = T\int_0^1 \left\{ \frac{\dot{x}^2}{2T^2} - \mathsf{v}[x,x'] \right\} dt, \quad (3)$$

where time, t, has been rescaled to make the period of the loops be 1. The equations of motion are given by stationarising the action with respect to changes in $x(t)$, keeping boundaries fixed, and phonons are (time) periodic solutions of the linearisation of these equations. Consider $S\left(x; \frac{2\pi}{\Omega}\right)$, where Ω is a potential phonon frequency and x now represents a period-1 loop in R^{Z}. To extend the renormalization method to study the phonon spectrum, $\mathcal{R}$ will now have to act on pairs of functionals $s\left(x, x'; \frac{2\pi}{\Omega}\right)$, so call an s-bond a τ or an υ according to the minimum energy case. The renormalization operator $\mathcal{R}$ can be extended (including one further scale, the phonon frequency scale) to

$$\mathcal{R}\left[(\tau,\upsilon)(x,x';\Omega)\right] = J\varepsilon\,(\upsilon\oplus\tau, \tau)\,(x/\alpha, x'/\alpha; \Omega/\varepsilon)\,. \quad (4)$$

where the operator $\oplus$ is

$$(\upsilon\oplus\tau)(x,x';\Omega) = \min_z\left[\upsilon(x,z;\Omega) + \tau(z,x';\Omega)\right], \quad (5)$$

and z now runs over period-1 functions $z(t)$.

Apart from the phonon spectrum scaling, ε, in the limit of $\Omega \to 0$ the operator is MacKay's minimum energy renormalization operator (applied pointwise to loops). It has therefore a fixed point in the $\Omega = 0$ subspace consisting of $\tau(x,x') = \int_0^1 dt\, \tau^*(x(t), x'(t))$ and $\upsilon(x,x') = \int_0^1 dt\, z\upsilon^*(x(t), x'(t))$. It was found numerically to have an additional unstable direction with eigenvalue [2] $\varepsilon = 1.649\,415$ (affecting the linearised dynamics), which we will call the Ω direction, whose origins we don't yet fully understand.

Thus the phonon spectrum (as a function of u,p) is asymptotically self-similar under scaling by ε, δ and η in the three directions (Ω, u, p). In particular the *phonon gap* (i.e. the minimum of the phonon spectrum) reduces by a factor ε when u approaches u_c by a factor δ from above along the curve $\rho =$ constant.

3 Quantum Effects

3.1 Zero temperature

The trace of the propagator for the lowest frequency phonons in the FK model is

$$\int \mathcal{D}\left[x\right] e^{\frac{i}{\hbar}\sum_n s\left(x_n, x_{n+1}; \frac{2\pi}{\Omega}\right)}, \tag{6}$$

where the Feynman functional integration is over closed loops and includes the endpoints. In stationary phase approximation (small $\hbar$) the integral is dominated by contributions of the stationary points of S; these are those functions which satisfy the classical equations of motion and are periodic with period T.

Consider pairs of functionals υ and τ as before, extend the operator $\oplus$ to non-zero $\hbar$ by

$$\left(\upsilon \oplus \tau\right)\left(x, x'; \Omega\right) = -i\hbar \log \int \mathcal{D}\left[z\right] e^{\frac{i}{\hbar}\left[\upsilon(x,z;\Omega)+\tau\left(z,x';\Omega\right)\right]}, \tag{7}$$

and extend also $\mathcal{R}$ to non-zero $\hbar$ with this new $\oplus$. It can be easily seen (keeping only the first terms in stationary phase) that in the limit $\hbar \to 0$ the operator $\oplus$ becomes the previous one for the phonon spectrum. If τ, υ and $\hbar$ are multiplied by a constant λ, then $\upsilon \oplus \tau$ is simply multiplied by the same constant λ, so the fixed point of the renormalization operator for the phonon spectrum extends to one at $\hbar = 0$ for this new $\mathcal{R}$ with a new unstable eigenvalue $\kappa = J\varepsilon \simeq 7.157\,051$ in the quantum direction. So the effect of including the quantum direction, close to the fixed point, is that $\mathcal{R}$ scales asymptotically like

$$\mathcal{R}\left(\tau, \upsilon\right)\left(\Delta u, \Delta p, \Omega^{-1}, \hbar\right) = \left(\tau, \upsilon\right)\left(\delta\Delta u, \eta\Delta p, \varepsilon\Omega^{-1}, \kappa\hbar\right), \tag{8}$$

for $\Delta u \equiv u - u_c$ and $\Delta p \equiv p - p_c\left(u\right)$ and $\Omega, \hbar$ small.

3.2 Statistical mechanics

The quantum partition function can be easily obtained from the trace of the quantum propagator by Wick rotation [3] (i.e. putting $T = -i\beta\hbar$ in equation (6)). The quantum partition function is then

$$Z\left(\beta, \hbar\right) = \int \mathcal{D}\left[x\right] e^{-\beta S_E(x;\beta\hbar)}, \tag{9}$$

where the Euclidean action S_E for the FK model is now the sum (instead of the difference) of the 'kinetic' and potential contributions. This gives another possible direction to which renormalization can be extended, the temperature direction, $\Theta = 1/\beta$. Redefine then the operator $\oplus$ by 'Wick rotating' the operator $\oplus$ for the trace of the propagator:

$$\left(\upsilon \oplus \tau\right)\left(x, x'; \beta, \hbar\right) = -\beta \log \int \mathcal{D}\left[z\right] e^{-\beta^{-1}\left[\upsilon(x,z;\beta\hbar)+\tau\left(z,x';\beta\hbar\right)\right]}, \tag{10}$$

Therefore, close to the fixed point of the associated renormalization operator, we have

$$\mathcal{R}\left(\tau, \upsilon\right)\left(\Delta u, \Delta p, \beta\hbar, \hbar\right) \sim \left(\tau, \upsilon\right)\left(\delta\Delta u, \eta\Delta p, \varepsilon\beta\hbar, \kappa\hbar\right), \tag{11}$$

so under the renormalization $\mathcal{R}$ there is a fixed point at $\hbar = 0$, $\beta\hbar = \infty$, with an unstable eigenvalue of $\kappa/\varepsilon = J \simeq 4.339\,143\,9$ in the temperature direction. This agrees with the result found by MacKay [4] for the classical statistical mechanics.

Acknowledgments

NRC was funded by the Portuguese institution 'Fundação para a Ciência e Tecnologia'.

References

1. S.Aubry & P.Y.Le Daeron, *Physica D* **8**, 381 (1983)
2. R.S.MacKay, *Physica D* **50**, 71 (1991)
3. J.W.Negele & H.Orland *Quantum Many-Particle Systems* (Perseus, 1998)
4. R.S.MacKay, *J. Stat. Phys.* **80**, 45 (1995)