Quantum Effects in the Frenkel-Kontorova Model

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We numerically study the quantized version of the Frenkel-Kontorova model, using Feynman quantization and the Metropolis algorithm. The gross structure of the quantum ground state above the critical parameter value mirrors the classical equilibrium configuration, provided that $\hbar$ is not too large; nevertheless, its fine structure is significantly different, and can be related to a sawtooth map rather than to the standard map. The dependence of energy on temperature is also investigated and is explained in terms of the quantum phonon spectrum for linearized motion.

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Much attention has been devoted in the last years to the properties of quantum systems which are classically described by nonintegrable maps. In the majority of cases, the analysis has been focused on *dynamical* problems, in which the maps describe the classical evolution in time of some physical model. In this connection great progress has been achieved in understanding the quantum relevance of classical nonintegrability, and some deep connections with problems of solid-state physics have been identified.[1] However, nonintegrable maps have important applications also in the study of *static* properties of condensed matter. The effect of quantization in such cases has been scarcely studied up to now.

The discrete Frenkel-Kontorova (FK) model is a well-known example in this class of problems.[2-5] Here the equilibrium configurations of a nonlinear chain of atoms are related to invariant curves or to invariant Cantor sets[6] which appear above a critical parameter value. The transition between these two states is called *transition by breaking of analyticity* (TBA). This is a deep change in the structure of the classical ground state occurring at some critical perturbation strength. This transition is accompanied by physically important phenomena, such as, e.g., the appearance of a *phonon gap*.[4] On account of the physical relevance of these classical predictions, it is important to assess what modifications of the classical picture of the FK model would be imposed by quantization.

We have therefore undertaken a numerical investigation of the quantum FK model. In this Letter we anticipate some new results which demonstrate that, above the critical parameter value, the quantum ground state exhibits significant differences from the classical picture.

The classical FK model is an infinite chain of linearly coupled harmonic oscillators in an external periodic potential. Its potential energy is given by

$$V=\sum_i \tfrac{1}{2}(x_i-x_{i-1})^2-K\cos(x_i)\,, \tag{1}$$

where x_i is the distance of the ith oscillator from a fixed position, and $K>0$ is the perturbative parameter. Particular attention has been given to the equilibrium positions of this model[2-4] and to the commensurate-incommensurate transition.[5] This phenomenon can be given a remarkable dynamical interpretation. Upon writing the conditions for V to be a minimum, and introducing new variables $p_{i+1}=x_{i+1}-x_i$ one finds that the equilibrium configurations satisfy

$$p_{i+1}=p_i+K\sin(x_i)\,,$$
$$x_{i+1}=x_i+p_{i+1}\,, \tag{2}$$

which means that these configurations are defined by orbits of the standard map.[7] Since this map exhibits a chaotic transition when K is increased, some kind of transition must be expected to occur also in the equilibrium configurations of the FK model. In the latter case one wishes to describe situations with a fixed density of atoms, which corresponds to selecting orbits of the standard map which have a given winding number ν. For small K and irrational ν these correspond to invariant tori [Kolmogorov-Arnol'd-Moser (KAM) curves]. These KAM curves break at some critical value of K. The destruction of the last KAM curve, which corresponds to the most irrational value of $\nu=(\sqrt{5}-1)/2$, occurs at $K_c=0.971\,635\ldots$. It can be shown[2,3] that for any irrational winding number there exists a *hull function* f which parametrizes the equilibrium positions [$u_i=x_i(\mathrm{mod}2\pi)$]

$$u_i=f((il+\alpha)(\mathrm{mod}2\pi))\,, \tag{3}$$

where α is an initial phase and l is the average unperturbed distance between two neighboring oscillators. This f can be a monotonic analytical function, or a monotonic function with a countable set of step discontinuities.[3,4] The transition between these two situations is just the above-mentioned TBA and can be numerically shown to occur at some critical value of K. Insofar as the dynamical properties of the standard map are con-

cerned, the existence of a discontinuous hull function proves the existence of cantori; instead, in the FK model it shows that the ground state of that model is never chaotic.

A number of critical effects accompany the TBA. For example, the phonon spectrum (i.e., the set of all frequencies of small oscillations around the equilibrium configuration) starts from 0 for $K<K_c$, but for $K>K_c$ there is a finite gap in it.[4]

In order to investigate the properties of the ground state in the quantum FK model, we consider a chain of s quantum oscillators with the potential (1), with a given length $2\pi r$ (r is an integer) and fixed ends, where r,s will be chosen so that r/s is a rational approximation to the irrational winding number $\nu=(\sqrt{5}-1)/2$. This is exactly the kind of approximation by means of periodic orbits which is used in numerical investigations of the destruction of KAM curves of the standard map. The results described below were obtained with r/s from 34/55 up to 233/377. The quantum Hamiltonian of our model is readily obtained from (1) and depends on the variables x_j, $1\le j\le s+1$, with $x_0=0$, $x_{s+1}=2\pi r$. We used Feynman quantization in Euclidean time. In this framework quantum thermodynamical quantities are given by appropriate averages over an ensemble of suitable weighted classical paths, taken over a Euclidean time τ. The parameter $T=\hbar\tau^{-1}$ plays the role of temperature. If T is small enough, the ground-state contribution is dominant and the ensemble average yields ground-state quantum expectation values.

In order to numerically compute this ensemble average we exploited the Metropolis algorithm.[8,9] This is well known and widely used in may areas of physics, and we shall not give details here; a full description of our numerical method will be given elsewhere. We shall just recall that this method performs an "importance sampling" by randomly generating a finite set of paths which mainly contribute in the Feynman integral. The actual number of paths needed for a satisfactory convergence of statistical averages depends on the number of time steps, which in turn must be large enough to isolate the ground-state contribution in the sum. We used ensembles from 2000 up to 8000 paths.

By this method we were able to compute the ground-state averages of the positions of the oscillators. The results thus obtained were compared with the classical equilibrium configuration in three ways: (1) We plotted the average positions $x_i(\mathrm{mod}2\pi)$ of the quantum oscillators against their unperturbed positions $(\mathrm{mod}2\pi)$. For the sake of simplicity, we call this plot a quantum hull function (QHF) (though this denomination may be abusive in a strict mathematical sense). (2) We computed

$$g_i=K^{-1}(x_{i+1}+x_{i-1}-2x_i) \tag{4}$$

and we plotted g_i against $x_i(\mathrm{mod}2\pi)$ for $i=1,\ldots,s$. In the classical case, the points thus obtained would lie in a Cantor subset of the graph of the function $g(x)=\sin(x)$ [Fig. 1(b)]. Again for the sake of simplicity we call this plot a g function (GF). (3) We plotted the points (x_i,p_i) in the phase space of the standard map. The results of such quantum computations are presented in Fig. 2. Some global characteristics of the classical case were found to persist; e.g., steps in QHF still exist [compare Fig. 2(c) with Fig. 1(a)]. However, the more detailed information supplied by the GF reveals significant changes. Quite remarkably, quantum fluctuations do not completely destroy the functional dependence of the g_i on $x_i(\mathrm{mod}2\pi)$, but change instead its shape to a sawtooth curve. In other words, the average positions of the oscillators in the quantum ground state appear to be approximately described by a sawtooth map rather than by the standard map. This is the more surprising in that the fluctuations of the positions of the oscillators are strongly

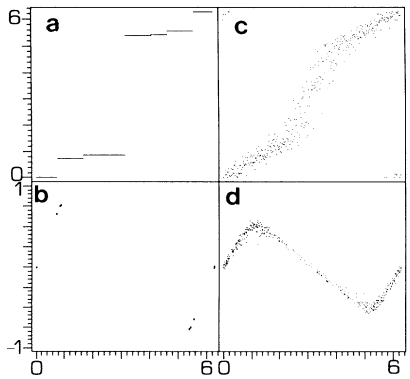

FIG. 1. Classical (a) hull function and (b) g function for winding number $\nu=233/377$, $K=5$; quantum (c) hull function and (d) g function, for the same ν and K, and $\hbar=3$.

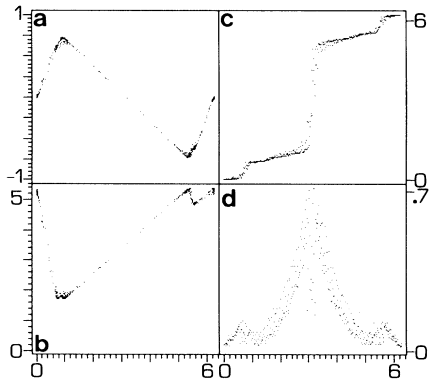

FIG. 2. Structure of the quantum ground state for K,ν as in Fig. 1 and $\hbar=0.2$ (a) g function, (c) hull function, (b) configuration in the phase space (x,p), (d) rms deviations of the positions of the quantum oscillators from their ground-state averages, plotted against the unperturbed position $(\mathrm{mod}2\pi)$.

correlated with their unperturbed positions [Fig. 2(d)]; these fluctuations are larger near the gap in the QHF. This is due to quantum tunneling between the edges of the gap. This tunneling produces double-peaked distributions of probability for the positions of the oscillators near the gap; such distributions were really observed in our computations. The appearance of a sawtooth-shaped GF has an interesting counterpart in the phase of the standard map. Here the quantum points spread out of the classical cantorus and tend to reduce the gaps in it; in doing so, they tend to dispose along straight lines connecting points of the cantorus. The resulting structure ("quantorus") looks much more like a curve than the classical ground state for the chosen parameter value; in any case the gaps in this quantum structure are significantly smaller than in the classical cantorus. It would be interesting to know whether and how this "curve" can be related to the phase-space structure of the above-mentioned sawtooth map, but the accuracy of our numerical results did not allow one to go very far in this direction. Of course the existence of quantum fluctuations makes it very likely that one cannot speak of invariant curves or cantori for the quantum ground state in a rigorous sense. Nevertheless, we believe that the concepts of QHF and GF provide an extremely convenient heuristic tool for the description of the quantum ground state. The above described changes in the properties of the ground state for finite $\hbar$ are not determined by temperature effects. This was checked by reducing the temperature in a few times. With the increase of $\hbar$, quantum fluctuations smoothen more and more the steps in the QHF; instead the GF keeps the same shape but with a lower amplitude [see Figs. 1(c) and 1(d)]. The monotonical decrease of the amplitude of GF continues also for larger values of $\hbar$; for example, for $K=5$, $\hbar=7$ the maximum of the GF is $\simeq 0.2$ while for $\hbar=0.2$ it is $\simeq 0.75$. In such cases the QHF becomes quite close to the diagonal. Finally, it is important to remark that the drastic change of the GF (from classical to quantum) takes place only above the critical value of K. Below that value the GF is still sine shaped, and only its amplitude changes, approaching zero for large $\hbar$.

Another important indication was provided by the study of the dependence on temperature T of the quantum average energy per oscillator $E(T)$. In computing the latter by the Metropolis algorithm, we used Feynman's prescription for kinetic energy.[8,9] A typical result is shown in Fig. 3. In order to analyze how the classical phonon spectrum (see, for example, Fig. 3 in Ref. 4) influences this dependence, we considered a quantum gas of noninteracting phonons associated with the frequencies of the classical linearized system. Having numerically computed these frequencies we could find $E(T)$ for such a gas. The *phononic* curves $E(T)$ thus found were compared with the Metropolis the data for the actual, nonlinear chain. We found a good agreement between

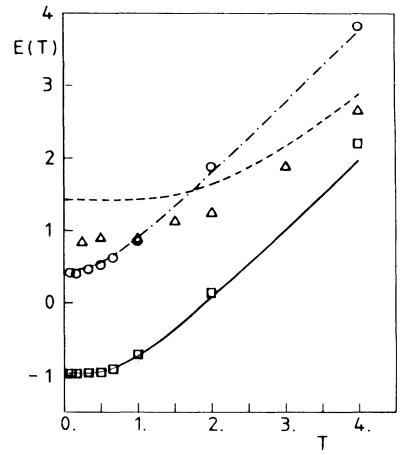

FIG. 3. Average energy per oscillator E vs temperature T for winding number $\nu=34/55$. The lines give $E(T)$ for the linearized chain; the symbols are the Metropolis data for the actual chain. Squares and full line: $\hbar=1$, $K=5$. Circles and dashed-dotted line: $\hbar=1$, $K=2$. Triangles and dashed line: $\hbar=3$, $K=5$.

the resulting *phononic* curves and the Metropolis data for different values of K and for not too large $\hbar$. An interesting feature is the initial plateau of almost constant energy (zero specific heat). This appears to be a quantum manifestation of the classical phonon gap, which sets a lower bound to the temperature required for significant excitation above the ground state. Nevertheless, when $\hbar$ is increased the phononic curve no longer fits the Metropolis points. A precise analysis of the behavior of $E(T)$ for such large $\hbar$ requires further investigations, which are now in progress.

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