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Quantum Frenkel-Kontorova model: A squeezed state approach

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The squeezed state is used to study the one-dimensional quantum mechanical Frenkel-Kontorova model. A set of coupled equations for the particle's expectation value and the fluctuations for the ground state are derived. It is shown that quantum fluctuations renormalize the standard map to an effective sawtooth map. The underlying mechanism provides an alternative and simple explanation of dynamical localization in quantum chaos. [S1063-651X(98)50610-1]

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The Frenkel-Kontorova (FK) model describes an atomic chain, connected by harmonic springs, subjected to an external sinusoidal potential. This model has been widely used to model the crystal dislocations [1], adsorbed epitaxial monolayers [2], and incommensurate structures [3]. The existence of two competing periodicities may lead to a rich behavior of the state configurational properties of the particles [4]. The application of the FK model to the study of transmission in Josephson junction and atomic-scale friction-nanoscale tribology, in which the quantum effects are very essential, has been witnessed in recent years [5].

For a deep understanding of the nanoscale tribology, it is very necessary to study the quantum FK model. However, in contrast to the classical FK model, up to now only a few works have been devoted to the effects of the quantum fluctuations in the FK model [6,7].

Like thermal fluctuations in classical systems at finite temperatures, quantum fluctuations play a very important role in quantum systems with finite $\hbar$. In particular, they become crucial and very important at zero temperature, when thermal fluctuations vanish. The study of quantum fluctuations becomes an important topic in quantum phase transitions [8] and quantum chaos.

Among many useful tools in study of quantum fluctuations, the squeezed state, which is a generalization of the coherent state, has been proven to be very useful in dealing with many-body problems [9,10]. In this Rapid Communication, we shall study the effect of quantum fluctuations in the one-dimensional FK model by using the squeezed state approach. As we shall see later, a set of coupled equations for the expectation value and the fluctuation of the particle will be derived for the ground state at zero temperature. We discover analytically how quantum fluctuations renormalize the external potential, which leads to the transition of the standard map in the classical FK model, to the sawtooth map in the quantum FK model. The results are found to be in good agreement with that of the quantum Monte Carlo (QMC) method.

The Hamiltonian operator of the one-dimensional standard FK model is

$$\hat{\mathcal{H}}=\sum_i \left[\frac{\hat{p}_i^2}{2m}+\frac{\gamma}{2}(\hat{x}_{i+1}-\hat{x}_i-a)^2-V\cos(q_0\hat{x}_i)\right]. \quad (1)$$

Here, m is the mass of particle, γ is the elastic constant of the spring, and $2\pi/q_0$ is the period of external potential. V is the strength of the external potential and a is the equilibrium distance between two nearest neighbor particles as the external potential vanishes. For convenience, we can rescale the variables into dimensionless ones and obtain a new Hamiltonian,

$$\hat{H}=\sum_i \left[\frac{\hat{P}_i^2}{2}+\frac{1}{2}(\hat{X}_{i+1}-\hat{X}_i-\mu)^2-K\cos(\hat{X}_i)\right], \quad (2)$$

where $K=Vq_0^2/\gamma$ is the rescaled strength of the external potential. The effective Planck constant $\tilde{\hbar}=\hbar(q_0^2/\sqrt{m\gamma})$, is the ratio of the natural quantum energy scale $(\hbar\omega_0)$ to the natural classical energy scale (γ/q_0^2), where $\omega_0^2=\gamma/m$.

The position and momentum operators for the ith particle are written as

$$\hat{X}_i=\sqrt{\frac{\tilde{\hbar}}{2}}\,(\hat{a}_i^\dagger+\hat{a}_i),$$
$$\hat{P}_i=i\sqrt{\frac{\tilde{\hbar}}{2}}\,(\hat{a}_i^\dagger-\hat{a}_i). \quad (3)$$

Here, $\hat{a}_i^\dagger$ and $\hat{a}_i$ are boson creation and annihilation operators, which satisfy the canonical commutation relations: $[\hat{a}_i,\hat{a}_j^\dagger]=\delta_{ij}$, $[\hat{a}_i,\hat{a}_j]=0$, and $[\hat{a}_i^\dagger,\hat{a}_j^\dagger]=0$.

The squeezed state $|\Phi\rangle$ is defined by the ordinary harmonic oscillator displacement operator $e^{\hat{S}(\alpha)}$ acting on a squeezed vacuum state,

$$|\Phi(\alpha,\beta)\rangle=e^{\hat{S}(\alpha)}e^{\hat{T}(\beta)}|0\rangle, \quad (4)$$

where

$$\hat{S}(\alpha)=\sum_i\,(\alpha_i\hat{a}_i^\dagger-\alpha_i^*\hat{a}_i),$$
$$\hat{T}(\beta)=\frac{1}{2}\sum_{ij}\,(\hat{a}_i^\dagger\beta_{ij}\hat{a}_j^\dagger-\hat{a}_i\beta_{ij}^\dagger\hat{a}_j). \quad (5)$$

$|0\rangle$ is the vacuum state and $\hat{a}_i|0\rangle=0$. $\hat{S}^\dagger(\alpha)=-\hat{S}(\alpha), \hat{T}^\dagger(\beta)=-\hat{T}(\beta)$. For simplicity, in what follows we will use the abbreviation $|\Phi\rangle=|\Phi(\alpha,\beta)\rangle$.

It must be noted that if we set $\beta=0$, the squeezed state is reduced to the coherent state. As we shall see later, the coherent state is not able to allow us to study the fluctuations.

Using $|\Phi\rangle$ as a trial wave function for Hamiltonian (2), we can easily find the expectation values of the coordinate and the momentum operators of the ith particle [9],

$$\overline{X_i}\equiv\langle\Phi|\hat{X}_i|\Phi\rangle=\sqrt{\frac{\tilde{\hbar}}{2}}\,(\alpha_i^*+\alpha_i),$$
$$\overline{P_i}\equiv\langle\Phi|\hat{P}_i|\Phi\rangle=-i\sqrt{\frac{\tilde{\hbar}}{2}}\,(\alpha_i^*-\alpha_i). \tag{6}$$

Fluctuations in the coordinate and the momentum are given by

$$\Delta X_i^2\equiv\langle\Phi|(\hat{X}_i-\overline{X_i})^2|\Phi\rangle=\tilde{\hbar}G_{ii},$$
$$\Delta P_i^2\equiv\langle\Phi|(\hat{P}_i-\overline{P_i})^2|\Phi\rangle, \tag{7}$$
$$=\tilde{\hbar}\left(\frac{G_{ii}^{-1}}{4}+4\sum_{l,k}\Pi_{il}G_{lk}\Pi_{ki}\right).$$

The fluctuation covariance between the ith particle and the jth particle is

$$\Delta X_i\Delta X_j\equiv\langle\Phi|(\hat{X}_i-\overline{X_i})(\hat{X}_j-\overline{X_j})|\Phi\rangle=\tilde{\hbar}G_{ij}, \tag{8}$$

where G_{ij} and Π_{ij} are

$$G_{ij}=\frac{1}{2}(\cosh^2\sqrt{\beta\beta^\dagger}+\sinh^2\sqrt{\beta\beta^\dagger})_{ij}+\frac{1}{2}(M\beta+\beta^\dagger M)_{ij},$$
$$\Pi_{ij}=\frac{i}{4}G_{ij}^{-1}(M\beta-\beta^\dagger M)_{ij}, \tag{9}$$

where

$$M=\frac{\sinh\sqrt{\beta\beta^\dagger}\,\cosh\sqrt{\beta\beta^\dagger}}{\sqrt{\beta\beta^\dagger}}. \tag{10}$$

Since β is a symmetric matrix, $G_{ij}=G_{ji}$ and $\Pi_{ij}=\Pi_{ji}$. Furthermore, using the following very important relation,

$$\langle\Phi|\cos\hat{X}_i|\Phi\rangle=\exp\left(-\frac{\tilde{\hbar}}{2}G_{ii}\right)\cos\overline{X_i}, \tag{11}$$

we can finally obtain the expectation value of the Hamiltonian $\hat{H}$,

$$\overline{H}\equiv\langle\Phi|\hat{H}|\Phi\rangle=\sum_i\frac{1}{2}\left[\overline{P_i^2}+\tilde{\hbar}\left(\frac{G_{ii}^{-1}}{4}+4\sum_{l,k}\Pi_{il}G_{lk}\Pi_{ki}\right)\right]$$
$$+\sum_i\frac{1}{2}(\overline{X}_{i+1}-\overline{X}_i-\mu)^2+\sum_i\frac{1}{2}[\tilde{\hbar}(G_{ii}+G_{i+1i+1})$$
$$-2\tilde{\hbar}G_{i+1i}]-\sum_i K\exp\left(-\frac{\tilde{\hbar}}{2}G_{ii}\right)\cos\overline{X}_i. \tag{12}$$

It is worth noting that the variables $\overline{X}_i$ and $\overline{P}_i$, and G_{ij} and Π_{ij} form explicitly canonical conjugates [10]. To find the ground state of the quantum FK model, we shall take a variational approach, and these four variables are regarded as variational variables. Variation with respect to $\overline{P}_i$ immediately yields $\overline{P}_i=0$ and, with respect to $\overline{X}_i$, yields

$$\overline{X}_{i+1}-2\overline{X}_i+\overline{X}_{i-1}=K_i\sin\overline{X}_i, \tag{13}$$

where $K_i=K\exp[-(\tilde{\hbar}/2)G_{ii}]$, which determines the expectation value of the particle's coordinate. Unlike its classical counterpart ($\tilde{\hbar}=0$, $K_i=K$), this equation is coupled with the quantum fluctuation by $\tilde{\hbar}G_{ii}$. Since we are considering the static problem, the variation with respect to Π_{ij} leads to $\Sigma_k G_{ik}\Pi_{kj}=0$. To obtain equation for G_{ij}, we first take the variation with respect to G_{ik} and note the following relation: $\delta G_{ij}/\delta G_{kl}=\delta_{ik}\delta_{jl}$, where δ_{ik} and δ_{jl} are Dirac δ functions. We then multiply both sides of the equation by G_{kj} and take the summation over k. Finally, we get the closed equations for the covariance G_{ij},

$$(GF)_{ij}=G_{i-1j}+G_{i+1j}, \tag{14}$$

where

$$F_{ij}=\delta_{ij}\left(1+\frac{K_i}{2}\cos\overline{X}_i\right)-\frac{(G^{-2})_{ij}}{8}. \tag{15}$$

This is a set of equations determining the quantum fluctuations of the particles $G=\{G_{ij}\}$. G is a $N\times N$ symmetric matrix that provides all the fluctuation information. Its diagonal elements give the variance of each particle, while its off-diagonal elements give the covariance between particles, from which we can calculate the correlation function of the quantum fluctuation. These equations are coupled with the expectation value $\overline{X}_i$.

Up to this point, we have obtained $N\times(N+1)/2+N$ equations for all variables. These equations provide a qualitative picture about the system before we proceed with any detailed numerical analysis. In fact, if we introduce a new variable, $I_{i+1}=\overline{X}_{i+1}-\overline{X}_i$, Eq. (13) can be cast into the map

$$I_{i+1}=I_i+K_i\sin\overline{X}_i,$$
$$\overline{X}_{i+1}=I_{i+1}+\overline{X}_i. \tag{16}$$

In the same manner, by denoting $Q_{i+1j}=G_{i+1j}-G_{ij}$, we can also write Eq. (14) into the form of a map

$$Q_{i+1j}=Q_{ij}+(G(F-2))_{ij},$$
$$G_{i+1j}=G_{ij}+Q_{i+1j}. \tag{17}$$

The difference between the classical ($\tilde{\hbar}=0$) and the quantum FK model is readily seen from Eq. (16). In the classical case the control parameter, namely, the amplitude of the external potential, does not change with the position index i. However, in the quantum case, due to the quantum fluctuation, the amplitude of the effective external potential, which acts on the particle, changes from particle to particle. Because $G_{ii}>0$, for any nonzero $\tilde{\hbar}$, $K_i<K$, which means that the quantum fluctuation reduces the external potential strength acting on the particle. Another important difference is that, in the classical case, the coordinates of the atoms in the ground state are determined by the standard map, whereas in the quantum case they are determined by $(N+1)$ coupled two-dimensional maps. This makes the quantum FK model extremely difficult to deal with analytically.

Before we turn to the numerical calculation, it is worth pointing out that in the case of $\beta=0$ in Eq. (4), $G_{ij}=\frac{1}{2}$ (for all $i,j=1,2,\ldots,N$), which is the result of the coherent state theory. It is obvious that this cannot be the case for a real quantum FK model. So, the coherent state is not suitable for the study of the quantum FK model.

We now make some comparisons with the quantum Monte Carlo (QMC) method. As mentioned before, finding the solution from two sets of equations [Eqs. (13) and (14)] is equivalent to finding the periodic orbit in a $2(N+1)$-dimensional map [Eqs. (16) and (17)]. This is still a big problem to be solved in nonlinear dynamics. Nevertheless, we can make a numerical test for Eq. (13) to see whether this equation can give rise to the ''sawtooth map'' [6].

In Fig. 1 we show the quantum Monte Carlo results (left column) and the results calculated from Eq. (13) (right column) by using the QMC's fluctuation data G_{ii} in the supercritical regime ($K=5$), with $\tilde{\hbar}=0.2$, for an incommensurate ground state. In our quantum Monte Carlo computation, as usual, we use the continued fraction expansion for the golden mean winding number $(\sqrt{5}-1)/2$. Thus, we use Q particles, which substrated into P external potentials, with a period of 2π. The periodic boundary condition is used (Ref. [11]): $\overline{X}_{Q+i}=\overline{X}_i+2\pi P$. The winding number is P/Q. The results shown in the figure are for $P/Q=34/55$.

By using the QMC calculation, we obtained the expectation value of the atom's coordinate, from which we can construct the so-called quantum Hull function, namely, $\overline{X}_i$ (mod 2π) versus the unperturbed $2\pi iP/Q$ (mod 2π), which is shown at top left in Fig. 1. The g function, which is defined by [6]

$$g_i\equiv K^{-1}(\overline{X}_{i+1}-2\overline{X}_i+\overline{X}_{i-1}), \tag{18}$$

is shown in the middle left of Fig. 1 from the QMC data. The quantum fluctuation G_{ii}, calculated from QMC, is shown also at the bottom-left of Fig. 1.

To compare the squeezed state results with those from QMC, we substitute G_{ii}, calculated from QMC, into Eq. (13), and then compute the expectation value of the particles' coordinates by using Aubry's gradient method. We then construct the quantum Hull function and the quantum g function, which is shown in the right-hand column of Fig. 1.

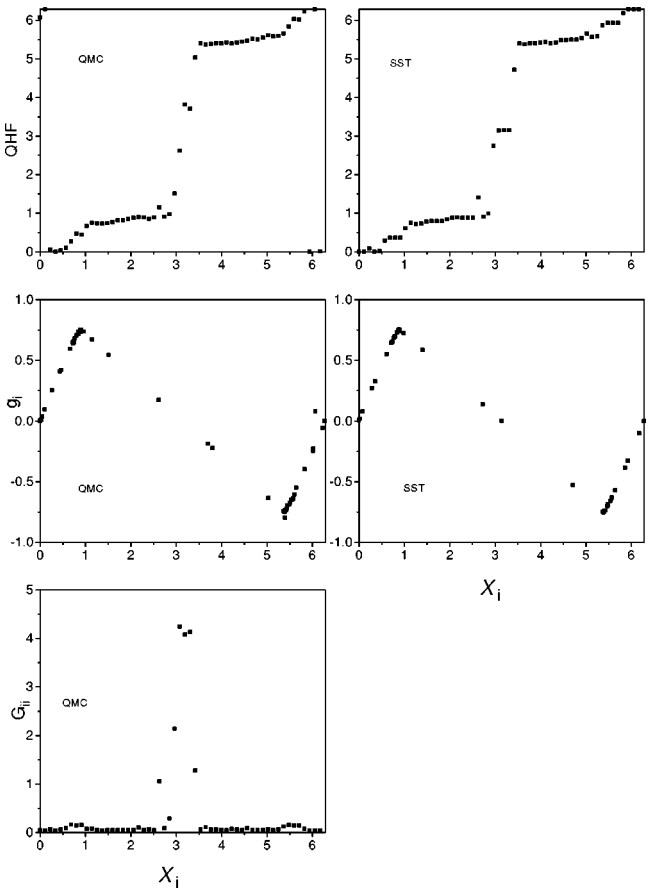

FIG. 1. Comparison between the quantum Monte Carlo (QMC) results (left-hand column) and the results from the squeezed state theory [Eq. (13), right-hand column] in the supercritical regime, where $K=5$, with $\tilde{\hbar}=0.2$. The abscissa is the average position of the particle (mod 2π) at zero external potential.

The results from Eq. (13) (right-hand column) agree surprisingly well with those from QMC for the quantum Hull function as well as the g function. The most striking feature to be noted is the sawtooth shape of the g function in the supercritical regime. This phenomenon was first observed by Borgonovi *et al.* [6] in their QMC computation, and has been explained as a tunneling effect. Later on, Berman *et al.* [7] recovered this phenomenon by using a mean field theory, including the contribution from quasidegenerate states. In the framework of the squeezed state theory, this quantum sawtooth map is just a straightforward result of Eq. (13), which results from the quantum fluctuations. Our result demonstrates that the squeezed state approach indeed captures the effects of quantum fluctuations.

Finally, we would like to point out that the mechanism of the reduction of the effective potential, due to the quantum fluctuations demonstrated above, can be applied to explain the quantum suppression of chaos and relevant phenomena, such as dynamical localization, in quantum chaos. The dynamical localization is a well-established fact, it was observed numerically by Casati *et al.* [12] almost 20 years ago, and was confirmed recently in several different experiments, such as hydrogen atoms in microwave fields, and so on [13]. Its underlying mechanism is still not completely understood.

Here, we shall demonstrate that by applying the squeezed state approach to the kicked rotator, we could obtain a simple and clear picture of the dynamical localization.

Using the squeezed state, we obtain a map, such as Eq. (16), for the expectation value of the angular variable and angular momentum. But the equation determining G_{ii} is different from Eq. (14); in this case it can be numerically calculated. We found that when the fluctuation G_{ii} grows quadratically with time (kicks), eventually the strength of external control parameter K_i becomes very small, thus the classical chaos is completely suppressed and leads to the dynamical localization. This gives us an alternative explanation and a very simple picture of the dynamical localization. In turn, it shows that the squeezed state is a very useful tool in the study of the phenomena related to the quantum fluctuations.

In conclusion, we have derived a set of coupled equations, determining the expectation values of the coordinate and the quantum fluctuations, by using the squeezed state as a trial wave function. The results from the squeezed state theory agree with those from the quantum Monte Carlo method quite well. Furthermore, the squeezed state results give us a very clear understanding of the renormalization of the standard map in the classical case to the effective sawtooth map in the quantum case. Moreover, the squeezed state approach provides an alternative and a simple picture of the dynamical localization observed in many quantum systems.

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