The 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 mechanism underlying provides an alternative and simple explanation of dynamical localization in quantum chaos.

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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 configurations [4]. Recent years have witnessed 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 [3].

To get 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 [5,6].

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 [3] 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 proved to be very useful in dealing with many-body problems [7,8]. In this Letter, 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 classical FK model to the sawtooth map in the quantum FK model. The results are found to be in a good agreement with that of quantum Monte Carlo (QMC) method.

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

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

(1)

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

\[
\hat{\mathcal{H}} = \sum_i \left[ \frac{\hat{p}_i^2}{2} + \frac{1}{2} (\hat{X}_{i+1} - \hat{X}_i - \mu)^2 - K \cos(\hat{X}_i) \right].
\]

(2)

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

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

\[
\hat{X}_i = \sqrt{\frac{\hbar}{2}} (\hat{a}_i^+ + \hat{a}_i), \quad \hat{P}_i = i \sqrt{\frac{\hbar}{2}} (\hat{a}_i^+ - \hat{a}_i)
\]

(3)

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

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

\[
|\Phi(\alpha, \beta)\rangle = e^{S(\alpha)} e^{T(\beta)} |0\rangle,
\]

(4)

where

\[
\hat{S}(\alpha) = \sum_i (\alpha_i \hat{a}_i - \alpha_i^* \hat{a}_i^+), \quad \hat{T}(\beta) = \frac{i}{2} \sum_{ij} (\hat{a}_i^+ \beta_{ij} \hat{a}_j^+ - \hat{a}_i \beta_{ij}^* \hat{a}_j^+).
\]

(5)

\( |0\rangle \) is the vacuum state and \( \hat{a}_i |0\rangle = 0 \). \( \hat{S}^+(\alpha) = -\hat{S}(\alpha), \hat{T}^+(\beta) = -\hat{T}(\beta) \). 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 $\hat{H}$, we can easily find the expectation values of the coordinate and the momentum operators of the $i$th particle, $\hat{X}_i, \hat{P}_i$:

$$X_i \equiv \langle \Phi | \hat{X}_i | \Phi \rangle = \sqrt{\frac{2}{\hbar}} (\alpha_i^+ + \alpha_i),$$

$$\hat{P}_i \equiv \langle \Phi | \hat{P}_i | \Phi \rangle = -i \sqrt{\frac{\hbar}{2}} (\alpha_i^+ - \alpha_i).$$

(6)

Fluctuations in the coordinate and the momentum are given by

$$\Delta X_i^2 \equiv \langle \Phi | (\hat{X}_i - \bar{X}_i)^2 | \Phi \rangle = \hbar G_{ii},$$

$$\Delta P_i^2 \equiv \langle \Phi | (\hat{P}_i - \bar{P}_i)^2 | \Phi \rangle,$n

$$= \hbar (G_{ii}^{-1} + 4 \sum_{i,k} \Pi_{il} G_{lk} \Pi_{ki}).$$

(7)

The fluctuation covariance between the $i$th and the $j$th particle is

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

where, $G_{ij}$, and $\Pi_{ij}$

are

$$G_{ij} = \frac{1}{2}((\cosh^2 \sqrt{\beta^2 + \sinh^2 \sqrt{\beta^2}})_{ij} + \frac{1}{2}(M_\beta + M_\beta^+ M)_{ij},$$

$$\Pi_{ij} = \frac{1}{2}G_{ij}^{-1}(M_\beta - M_\beta^+ M)_{ij},$$

(9)

where,

$$M = \frac{\sinh \sqrt{\beta^2 + \cosh \sqrt{\beta^2}}}{\sqrt{\beta^2 + \cosh \sqrt{\beta^2}}}.$$  

(10)

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

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

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

$$\hat{H} \equiv \langle \Phi | \hat{H} | \Phi \rangle = \sum_i \frac{1}{2} \left( \hat{P}_i^2 + \hbar (G_{ii}^{-1} + 4 \sum_{i,k} \Pi_{il} G_{lk} \Pi_{ki}) \right)$$

$$+ \sum_i \frac{1}{2} (\bar{X}_{i+1} - \bar{X}_i - \mu)^2 \tag{12}$$

$$+ \sum_i \frac{1}{2} \left( \hbar (G_{ii} + G_{i+1i+1}) - 2\hbar G_{ii+1} \right)$$

$$- \sum_i K \exp \left( -\frac{\hbar}{2} G_{ii} \right) \cos \bar{X}_i,$$

(13)

where $K_i = K \exp \left( -\frac{\hbar}{2} G_{ii} \right)$, which determines the expectation value of the particle’s coordinate. Unlike its classical counterpart ($\hbar = 0$, $K_i = K$), this equation is coupled with the quantum fluctuation by $\hbar G_{ii}$. Variation w.r.t. $\Pi_{ij}$ leads to $4\hbar G_{ij} \Pi_{ji} = 0$. Since the fluctuation $G_{ij}$ cannot be zero, they are always positive, we have $\Pi_{ji} = 0$. To obtain equation for $G_{ij}$, we first take variation w.r.t. $G_{ik}$ and note the following relation:

$$\frac{\delta G_{ij}}{\delta G_{ik}} = \delta_{ik}\delta_{ij},$$

where, $\delta_{ik}$ and $\delta_{ji}$ are Dirac delta functions. We then multiply both sides of the equation by $G_{kj}$ and take 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

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

This is a set of equations determining the quantum fluctuations of the particles, $G = \{G_{ij}\}$. $G$ is a $N \times N$ symmetric matrix which 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 $\bar{X}_i$.

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 to do any detailed numerical analysis. In fact, if we introduce a new variable, $I_{i+1} = X_{i+1} - X_i$, Eq. (13) can be cast into the map,

$$I_{i+1} = I_i + K_i \sin X_i,$$

$$\bar{X}_{i+1} = I_{i+1} + \bar{X}_i. \tag{16}$$

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 ($\hbar = 0$) and the quantum FK model from Eq. (16) is readily seen. 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 $\hbar$, $K_i < K$, 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-dimension 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.(1), $G_{ij} = 1/2$ (for all $i, j = 1, 2, \cdots, N$), 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, coherent state is not suitable for the study of quantum FK model.

We now make some comparisons with the quantum Monte Carlo (QMC) method. As mentioned before, to find the solution from two sets of equations Eqs. (14) and (15) is equivalent to find the periodic orbit in a $2(N + 1)$-dimensional map Eq.(16) and Eq.(17). This is still a big problem in the nonlinear dynamics to be solved. Nevertheless, we can make a numerical test of the Eq.(13) to see whether this equation can give rise to the "sawtooth map".

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 $\hbar = 0.2$ 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 period of $2\pi$. Periodic boundary condition is used: $\bar{X}_{Q+i} = \bar{X}_i + 2\pi P$. The winding number is $P/Q$. The results shown in the figure is for $P/Q = 34/55$.

By using QMC calculation, we obtained the expectation value of the atom’s coordinate, from which we can construct the so called quantum Hull function (QHF), namely $\bar{X}_i$ (mode $2\pi$) versus the unperturbed ones $2\pi P/Q$ (mode $2\pi$), which is shown in top-left in Fig. 1.

The $g$-function which defined by

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

is shown in the middle-left of Fig. 1 from the QMC data. The quantum fluctuation $G_{ii}$ calculated from QMC is shown also in 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 quantum $g$-function, which is shown in the right column of Fig. 1.

The results from Eq.(13) (right 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 Borgenovoi et al. in their QMC computation and has been explained as a tunneling effect. Later on Berman et al. 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 correctly and nicely 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 suppresion of chaos and relevant phenomena such as dynamical localization in quantum chaos. The dynamical localization is a well-established fact, it was observed by Casati et al. [4] numerically almost 20 years ago and confirmed recently in several different experiments such as hydrogen atoms in microwave fields and so on [5]. 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 like Eq. (14) 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 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 study the phenomena related with 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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