Ground state wavefunction of the quantum Frenkel-Kontorova model

BAMBI HU\textsuperscript{1}(∗) AND BAOWEN LI\textsuperscript{1}\textsuperscript{(**)}

\textsuperscript{1}Department of Physics and Centre for Nonlinear Studies, Hong Kong Baptist University, Hong Kong, China
\textsuperscript{2}Department of Physics, University of Houston, Houston TX 77204-5506, USA

(received ; accepted )

PACS. 64.70 Rh− .
PACS. 64.70.−p− .

Abstract. – The wavefunction of an incommensurate ground state for a one-dimensional discrete sine-Gordon model – the Frenkel-Kontorova (FK) model – at zero temperature is calculated by the quantum Monte Carlo method. It is found that the ground state wavefunction crosses over from an extended state to a localized state when the coupling constant exceeds a certain critical value. So, although the quantum fluctuation has smeared out the breaking of analyticity transition as observed in the classical case, the remnant of this transition is still discernible in the quantum regime.

The Frenkel-Kontorova (FK) model was proposed more than half a century ago to study commensurate-incommensurate phase transitions [1]. It has since become a widely used model not only in condensed matter physics but also in nonlinear dynamics (see e.g. [2]). In condensed matter physics, it serves as a model for an adsorbate layer on the surface of a crystal [3, 4], ionic conductors and glassy materials [5], charge-density waves [6], and chains of coupled Josephson junctions [7]. Moreover, the FK model is also a nonlinear lattice model having a normal thermal conduction [8]. Recently there has been a growing interests in applying this model to study dry-friction [9] and atomic scale friction or nanotribology [10]. In nonlinear dynamics, the FK model provides a vivid physical realization of the seminal Kolmogorov-Arnol’d-Moser theorem.

The FK model describes a chain of particles connected by harmonic springs and subject to an external sinusoidal potential. The classical behavior of this model has been studied by Aubry [3]. As a discrete sine-Gordon model, the FK model exhibits many new features that are absent in the continuum sine-Gordon model. One of the most striking features is the so-called “breaking of analyticity” transition. In an incommensurate ground state, as the
coupling constant increases beyond a critical value, the FK model displays a transition between the unpinned state (sliding phase) and the pinned state (pinned phase). This transition is characterized by the appearance of a phonon gap, the discontinuity of the Hull function, and etc. [3]. These phenomena have been also found in many generalized FK models [11].

Although a lot of studies have been done on the classical FK model, very little study has been devoted to the quantum FK model [12, 13, 14, 15]. Such study is also of more than academic interest. For example, recently there has been a surge in the study of atomic scale friction, or nanotribology. This problem is of tremendous importance to technology. The FK model has been used to study this problem. However, in the nano-regime, it’s inevitable that quantum mechanics will play an important role. So an understanding of the quantum FK model will be important to the understanding of nanotribology.

In this Letter we would like to study the quantum version of the one dimensional FK model by using the quantum Monte Carlo approach. We shall concentrate on the wavefunction of an incommensurate ground state. As we shall see later the wave function changes from an extended state to a localized one as the coupling constant is increased beyond a certain critical value. This crossover is a quantum remnant of the classical breaking of analyticity transition.

The Hamiltonian operator of the one dimensional 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 the particles, \(\gamma\) the elastic constant of the spring, \(2\pi/q_0\) the period of the external potential, \(V\) the magnitude of the external potential, and \(a\) the equilibrium distance between two nearest neighbor particles. For convenience, we shall rescale the variables so as to obtain a dimensionless Hamiltonian

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

(2)

where \(K = Vq_0^2/\gamma\) is the coupling constant. We define an “effective Planck’s constant”:

\[\tilde{\hbar} = \hbar \frac{q_0^2}{\sqrt{m\gamma}}.\]  

(3)

This effective Planck’s constant is the ratio of the natural quantum energy scale \((\hbar \omega_0)\) to the natural classical energy scale \((\gamma/q_0^2)\) [14], and \(\omega_0^2 = \gamma/m\).

To study the ground state of Hamiltonian (2), the quantum Monte Carlo method will be employed [16]. As in the classical case, we will concentrate our attention on the incommensurate state characterized by the golden mean value \(\sigma_G = (\sqrt{5}-1)/2\). In the classical case the winding number is defined as the average separation of atoms per period, i.e. \(\sigma = \lim_{N \to \infty} \frac{X_N - X_0}{2\pi N}\). If \(\sigma\) is a rational number, the ground state is commensurate, and if it is an irrational number the ground state is called incommensurate. In the quantum case, \(X_i(i = 0, 1, \ldots, N)\) is defined as the expectation values of the particles. As usual, we use the method of continued fraction expansion and approximate \(\sigma_G\) by its rational convergents \(\sigma_G = F_n/F_{n+1}\), where \(F_n\) is the \(n\)th Fibonacci number defined by the recursion relation, \(F_{n+1} = F_n + F_{n-1}\) with \(F_0 = 0, F_1 = 1\). Therefore, in our quantum Monte Carlo computation, we choose \(F_{n+1}\) particles which are embedded into \(F_n\) external potentials with period of \(2\pi\). We impose periodic boundary condition on the chain.

Since the external potential is periodic and has period \(2\pi\), we can fold the wavefunction to this period and then take the average over all particles in the interval \([0, 2\pi]\). This quantity gives the probability of finding particles at a given potential position \(X\). We plot
the averaged probability density $\langle |\Psi|^2 \rangle$ in Fig. 1 with 144 particles embedded in 89 potentials for a fixed $\hbar (=0.2)$ for different values of $K$. (Notice that $\langle |\Psi|^2 \rangle$ is normalized, namely, $\int_0^{2\pi} dX \langle |\Psi(X)|^2 \rangle = 1$.) We observe that, in the small $K$ regime, the probability of finding the particles at any place of the potential is almost the same (see the curve for $K = 0.1$). This is quite similar to the sliding phase in the classical version. However, as the coupling constant increases, the probability of finding the particle at the top of the potential decreases, while that at the lower part of the potential increases, as is noticeable from the appearance of peaks in the curves. As the potential goes beyond a certain critical value, the probability of finding the particles at the top is almost zero, see e.g. the curves for $K = 2$ and 5.

In the classical FK model, Coppersmith and Fisher [18] have proposed a “disorder parameter” to describe the transition from the pinned phase to unpinned phase. This parameter is defined as the minimum distance of a particle from the top of a well, $D_{cl} = \min_{j,n} |X_j^q - 2\pi(n + \frac{1}{2})|$. It can be seen that, as long as $D_{cl} \neq 0$, the particles are pinned, while $D_{cl} = 0$ corresponds to an unpinned state. This “disorder parameter” also measures the discontinuity (or width of the biggest gap) of the Hull function. One might naively try to use the same function to describe the quantum crossover. For instance, one may define a very similar quantum disorder parameter $D_q = \min_{j,n} |X_j^q - 2\pi(n + \frac{1}{2})|$, where $X_j^q$ is the expectation value of the $j^{th}$ particle’s position. However, this parameter $D_q$ could not capture the crossover of the ground state wavefunction. The reason is that, in the quantum case, the particle can tunnel from one side of the potential to the other, thus the gap in the classical Hull function does not survive the quantum fluctuations (see Refs. [13] and [15]). It turns out that even if $K > K^q_c$, $D_q$ might be also close to (or equal to) zero. Therefore, a new parameter is needed to describe the wavefunction crossover in the quantum FK model. To this end, we define the probability of finding particles at the potential top as a quantum “disorder parameter”, which is denoted as $P_t$. $P_t$ is given by

$$P_t = \frac{1}{N} \sum_{n=0}^{N-1} \int |\Psi(X)|^2 \delta \left( X - 2\pi(n + \frac{1}{2}) \right) dX. \quad (4)$$

In Fig. 2(a)-(b) we plot $P_t$ versus $K$ for different temperature and different system size. In Fig. 2(a), we fix the quantum fluctuation $\hbar (= 0.2)$, and the particle numbers (13/21) by changing the temperature from $T_c = 0.2/30, 0.2/120$, to $0.2/480$. The convergence is quite fast as is seen from the figure. The sharp decrease of $P_t$ is very evident for $K$ between 1 and 2. In this small $K$ regime, $P_t$ changes dramatically: it drops almost two orders of magnitude. This dramatical change can also be seen from Fig.2 (b). There the temperature is fixed at $T_c = \hbar/N\delta \tau = 0.2/120$, which can be regarded as effectively zero temperature. The system size is changed from 21 particles to 144 particles. In the quantum Monte Carlo method the Feynman path integral presentation is used. In this presentation, solving a one dimensional quantum problem is equivalent to solving a two dimensional effective classical problem with an extra dimension as the imaginary time $\tau$. The size of this extra dimension is $\hbar \beta$, where $\beta = 1/T_c$. $T_c$ is the temperature. Therefore, in the zero temperature limit, we shall take $\beta$ infinite.

It is worth pointing out that another parameter which can be used to depict this crossover is the maximal fluctuations of the particles. In the quantum case, we have observed that the particle situated at a position nearest to the maxim of the potential has always maximal fluctuation since it has the largest classical potential energy. This observation has been verified numerically by the quantum Monte Carlo results, and theoretically by our squeezed state theory [15]. Thus, we can use this maximal fluctuation as another measure of quantum “disorder”. To make a qualitative comparison with the classical disorder parameter $D_{cl}$, defined
Fig. 1. – The wavefunction of an incommensurate ground state having winding number 89/144 at fixed $\tilde{\hbar} = 0.2$ for different values of $K$. The wavefunction $\langle |\Psi|^2 \rangle$ means the probability of finding the particles at $X$ (mod $2\pi$). The curves are for $K = 0.1, 1, 2,$ and $5$, respectively. The wavefunction becomes localized at the lower part of the potential as $K$ changes to 2 and 5.

by Coppersmith and Fisher [18], we shall make use of the standard deviation, i.e. the square root of the maximal fluctuation,

$$
\Delta = \max_j \left\{ \left( \langle X_j^2 \rangle - \langle X_j \rangle^2 \right)^{1/2} \right\}.
$$

Here the average $\langle \cdots \rangle$ is taken over all the paths produced in the quantum Monte Carlo simulation, which is about 4,000 in our calculations. $\Delta$ versus $K$ is plotted in Fig. 3. The computations given in this figure have been carried out with $\sigma = F_n/F_{n+1} = 34/55$.

It is noticeable that the transition of the wavefunction is characterized by the different $K$-dependent behavior of $\Delta$. For $K < K_q^*$, $\Delta$ is a constant. It does not depend on $K$, but it changes with $\tilde{\hbar}$. For $K > K_q^*$, the maximal fluctuation increases with $K$, but it does not change with $\tilde{\hbar}$. Furthermore, this quantum parameter $\Delta$ is approximately equal to the classical disorder parameter $D_{cl}$. For comparison with the classical disorder parameter, we also include $D_{cl}$ in the inset of Fig. 3. In the classical case, the transition occurs at $K = K_c^*$, where $K_c^* = 0.971635 \ldots$.

These results show that the width and the shape of the probability density do not change by changing the external potential strength in the small $K(< K_q^*)$ regime. The width only depends on the strength of the quantum fluctuation $\tilde{\hbar}$. However, this picture changes dramatically when $K > K_q^*$. In this regime, the profile of the probability density spreads out, and the width of the probability density is insensitive to quantum fluctuations; instead it depends only on the coupling constant. It must be stressed that the analogy between $D_{cl}$ and $\Delta$ cannot be carried too far, since $\Delta$ is not exactly the quantum correspondence of $D_{cl}$. This is why even if we let $\tilde{\hbar}$ go to zero, $\Delta$ would not be zero in the regime of $K < K_q^*$.

In summary, we have studied the ground state wavefunction of the FK model at zero temperature. The wavefunction undergoes a crossover from an extended state (analogous to the sliding phase) to a localized state (analogous to the pinned phase) as the external potential increases. Therefore, although the quantum fluctuation has smeared out the breaking of analyticity transition as observed in the classical case, the remnant of this transition is still discernible in the quantum regime.

***

We would like to thank S. Aubry, F. Borgonovi, D. K. Campbell, H. Chen, R. B. Griffiths, H.-Q. Lin, L.-H. Tang, and W.-M. Zhang for helpful discussions during several periods of the work. BL thanks the Abdus Salam International Centre for Theoretical Physics (Trieste) for its kind hospitality during his visit there in the summer of 1998. This work was supported in part by the grants from the Hong Kong Research Grants Council (RGC) and the Hong Kong Baptist University Faculty Research Grant (FRG).

**Figures. –**

REFERENCES
Fig. 2. – The quantum “disorder parameter” $P_t$, i.e. the probability of finding particles on the top of the external potential versus $K$ for a fixed quantum fluctuation $\hbar = 0.2$. (a) $P_t$ for different temperature at a fixed winding number 13/21. The temperature changes from 0.2/30, 0.2/120, and 0.2/480, respectively. (b) $P_t$ for different winding numbers: 13/21, 34/55, and 89/144, at fixed temperature $T = 0.2/120$, which can be effectively regarded as zero.

Fig. 3. – $\Delta$ versus $K$. Different symbols represent different effective Planck's constant, which are $\hbar = 0.01$, and 0.1, respectively. We draw the classical disorder parameter defined by Coppersmith and Fisher [17] in the inset for comparison. The winding number for all calculations given in this figure is 34/55.

[1] Frenkel Y and Kontorova T K, Zh. Eksp. Teor. Fiz., 8 (1938) 1340; Frank F and van der Merwe J, Proc. R. Soc. London A, 198, 205 (1949) 205.
[2] Bak P, Rep. Prog. Phys., 45 (1982) 587 and references therein; Selke W, in Phase Transition and Critical Phenomena, ed. Domb C and Lebowith J L., Vol. 15. Academic Press 1992, London.
[3] Aubry S, in Solitions and Condensed Matter Physics., edited by Bishop A R. and Schneider T., (Springer, New York, 1978; Aubry S, J. Phys. (France), 44 (1983) 147; Peyrard M and Aubry S, J. Phys. C, 16 (1983) 1593; Aubry S, Physica D, 7 (1983) 240; Aubry S and Le Daëron P Y, ibid 8 (1983) 381.
[4] Uihler W and Shilling R, Phys. Rev. B, 37 (1988) 5758.
[5] Pietronero L, Schneider W R, and Strassler S, Phys. Rev. B, 24 (1981) 2187; Aubry S, J. Phys. (France), 44 (1983) 147; Vallet F, Schilling R, and Aubry S, J. Phys. C, 21 (1988) 67.
[6] Floria L M and Mazo J J, Adv. Phys., 45 (1996) 505.
[7] Watanabe S, van der Zant H S J, Strömgård S H, and Orlando T P, Physica D, 97 (1996) 429.
[8] Hu B, Li B, and Zhao H, Phys. Rev. E, 57 (1998) 2992 ; Fillipov A, Hu B, Li B, and Zeltser A, J. Phys. A, 31 (1998) 7719 ; Tong P.-Q, Li B, and Hu B, Phys. Rev. B, 59 (1999) 8639.
[9] Braun O M, Dauxois T, Paliy M V, and Peyrard M, Phys. Rev. Lett., 78 (1997) 1295; Phys. Rev. E, 55 (1997) 3598; Braun O M, Bishop A R, and Röder J, Phys. Rev. Lett., 79 (1997) 3692. Weisse M and Elmer F J, Phys. Rev. B, 53 (1996) 7539; Stunz T and Elmer F J, Phys. Rev. E, 58 (1998) 1602, 1612; Zheng Z G, Hu B, and Hu G, Phys. Rev. B, 58 (1998) 5453.
[10] Rozman M G, Urbakh M, and Klafter J, Phys. Rev. Lett., 77 (1996) 683; Zaloj V, Urbakh M, and Klafter J, Phys. Rev. Lett., 81 (1998) 1227.
[11] Johannesson H, Schaub B and Suh H, Phys. Rev. B, 37 (1988) 9625; Lin B and Hu B, J. Stat. Phys., 69 (1992) 1047; Shi J and Hu B, Phys. Rev. A, 45 (1992) 5455; Chou C I, Ho C L, and Hu B, Phys. Rev. E, 55 (1997) 5092; Chou C I, Ho C L, Hu B, and Lee H, ibid. 57 (1998) 2747; Xu A G, Wang G R, Chen S G, and Hu B, Phys. Rev. B, 58 (1998) 721; Xu A G, Wang G R, Chen S G, and Hu B, Phys. Rev. B, 57 (1998) 2771.
[12] Bak P and Fukuyama H, Phys. Rev. B, 21 (1980) 3287.
[13] Borgonovi F, Guarneri I and Shepeliansky D, Phys. Rev. Lett., 63 (1989) 2010; Z. Phys. B, 79 (1990) 133; Borgonovi F., Ph. D dissertation., Università Degli Studi di Pavia, 1989, Italia.
[14] Berman G P, Bulgakov E N and Campbell D K, Phys. Rev. B, 49 (1994) 8212.
[15] Hu B, Li B, Zhang W M, Phys. Rev. E, 58 (1998) R4068.
[16] Creutz M and Freedman B, Ann. Phys., 132 (1981) 472; Shuryak E V and Zhitov O V, Nucl. Phys. B, 242 (1984) 393.
[17] Sondhi S L, Girvin S M, Carini J P, and Shahar D, Rev. Mod. Phys., 69 (1997) 315.
[18] Coppersmith N and Fisher D S, Phys. Rev. B, 28 (1983) 2566.
$\Delta$ vs $K$

Inset: $D_{c1}$ vs $K$