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Mode-locking of incommensurate phase by quantum zero point energy in the Frenkel-Kontorova model

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Abstract. – In this paper, it is shown that a configuration modulated system described by the Frenkel-Kontorova model can be locked at an incommensurate phase when the quantum zero point energy is taken into account. It is also found that the specific heat for an incommensurate phase shows different parameter-dependence in sliding phase and pinning phase. These findings provide a possible way for experimentalists to verify the phase transition by breaking of analyticity.

The Frenkel-Kontorova (FK) model was proposed to study successive commensurate-incommensurate phase transitions observed in many configuration modulated systems such as low-dimensional conductors having charge density waves and some ferroelectric materials (see recent review [1]). It has also been used widely to study transmission in Josephson junction and atomic-scale friction -nanoscale tribology [2, 3]. More recently, this model has been employed to study transport properties of vortices in easy flow channels[4] and strain-mediated interaction of vacancy lines in a pseudomorphic adsorbate system[5].

The FK model consists of a chain of particles having nearest-neighbor harmonic interaction and adsorbed in an external periodic potential. The Hamiltonian of the FK model is

$$\mathcal{H} = \sum_i \left[\frac{p_i^2}{2m} + \frac{\gamma}{2} (x_{i+1} - x_i - a)^2 - \frac{V}{(2\pi)^2} \cos \frac{2\pi x_i}{b} \right], \quad (1)$$

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which can be cast into a dimensionless one

$$H = \sum_i \left[\frac{P_i^2}{2} + \frac{1}{2}(X_{i+1} - X_i - \mu)^2 - \frac{k}{(2\pi)^2} \cos 2\pi X_i \right], \quad (2)$$

where P_i and X_i are the dimensionless classical momentum and position of the i th particle, $k = \frac{V}{b^2\gamma}$ is a dimensionless coupling constant and μ the dimensionless lattice constant at vanishing k . The most important quantity of interest is the ratio (ρ) of the mean distance between neighboring particles and the period of the external periodic potential (one)

$$\rho = \lim_{N \rightarrow \infty} \frac{X_N - X_0}{N}. \quad (3)$$

Because the competition between two length scales the FK model exhibits abundant interesting phenomena [1, 6, 16]. Among many others is the mode-locking which manifests itself in the ‘devil’s staircase’ [6], i.e., the dependence of ρ on μ is described by a highly pathological function. Namely, $\rho(\mu)$ has the property that for all rational number ν , there exist real numbers $\mu(\nu_-)$ and $\mu(\nu_+)$ such that $\rho(\mu) = \nu$ if $\mu(\nu_-) < \mu < \mu(\nu_+)$. These mode-locking intervals show up as horizontal plateaus in $\rho(\mu)$. The widths of the plateaus are determined by the Farey sequence, i.e. the widest plateau between two plateaus at $\rho = p/q$ and $\rho = p'/q'$ is the plateau at $\rho = (p+p')/(q+q')$, where p/q and p'/q' are rational fractions. Accordingly, one can construct the Farey tree of the rationales with successive order starting from 0/1 and 1/1. Therefore, assuming k is a temperature- and pressure-dependent parameter, the model will exhibit a lock-in commensurate phase at relatively high order by changing temperature and/or pressure. This mechanism has been used to explain experimental results observed in thiourea [7] and in epitaxial thin film [8].

However, to obtain a reasonable and more accurate result one should consider quantum effect, in particular in low temperature regime. This problem becomes more and more important when people starting working on nano systems at very low temperature such as nano-tribology. One may ask: What happens to the commensurate and incommensurate mode-locking when the quantum effect is taken into account. In other words, can devil’s staircase survive the quantum fluctuations? This is not clear up to now. In fact, we have only limited knowledge coming from the continuum model, i.e. the sine-Gordon model, which is valid only for very small k . In the continuum limit, Bak and Fukuyama [9] discussed the local stabilities of the commensurate phases. They found that quantum effect would destroy the normal mode-locking staircase if the quantum fluctuation is large enough. However, for a more general case of k the picture is still incomplete.

On the other hand, the study of Borgonovi *et al* [11] by using the quantum Monte Carlo method shown that the quantum fluctuations, similar to the thermal fluctuations [10], smears out the discontinuity of hull function in classical FK model. One of the significant results is that the quantum effects, mainly from tunneling, renormalize the standard map to an effective sawtooth map. This phenomenon was also recovered by Berman *et al* [12] by using the method of mean-field theory and Hu, Li and Zhang [13] by using the squeezed state approach. Moreover, Hu and Li [14] found that although the quantum effects smear out the breaking of analyticity transition, the remnant of this transition is still discernible in the quantum FK model, which is demonstrated by the crossover of the ground state wave function from an extended one to a localized one as the coupling constant is increased. The transition also shows up in other relevant parameters [15].

In this paper we concentrate on effect of quantum zero point energy. The other effects such as quantum tunneling will be neglected. This approximation is valid provided that \hbar is not too large [11, 14]. As we will see soon that the quantum zero point energy can lead to interesting

results. For small k , all the commensurate phases seem to be destroyed. This agrees with Bak and Fukuyama's finding[9]. For large k the situation becomes more complex. The plateaus can be destroyed and enhanced depending on the system's parameters. More interestingly, for suitable scale of the quantum effect⁽¹⁾ the system may be locked into incommensurate phases. This mode-locking of incommensurate phase has a very special meaning in laboratory experiment.

In the low temperature regime, we assume that the quantum effect just causes the particle a small fluctuation around its equilibrium position. The phonon spectrum is calculated by linearizing the system around its equilibrium configuration, it is determined by

$$\mathbf{B} - \omega^2 \mathbf{I} = 0, \quad (4)$$

where \mathbf{B} is a constant matrix with elements

$$B_{ij} = \frac{\partial^2 H}{\partial X_i \partial X_j},$$

and \mathbf{I} is a unit matrix. The ground state energy is considered as the classical ground state energy plus the quantum zero point energy:

$$f = v_0 + f_0 \quad (5)$$

where

$$v_0 = \frac{1}{N} \left[\sum_{i=1}^N \frac{1}{2} (X_{i+1}^e - X_i^e - \mu)^2 - \frac{k}{(2\pi)^2} \cos 2\pi X_i^e \right], \quad (6)$$

is the classical ground state energy and

$$f_0 = \frac{1}{N} \sum_{l=1}^N \frac{1}{2} \omega_l \quad (7)$$

the quantum zero point energy at the ground state. Here X_i^e is the equilibrium position of i 'th particle in classical ground state. In Eq. (5) v_0 is measured in unit of $b^2\gamma$ while f_0 in unit of $\hbar\omega_0$, where $\omega_0^2 = \gamma/m$ and \hbar is the Plank constant. Thus the ratio $\tilde{\hbar} = \frac{\hbar\omega_0}{b^2\gamma}$ is a measure of the quantum zero point energy.

Throughout this paper, except special indication, 600 particles with periodic boundary condition were used in our numerical calculation. Since the system is symmetric about $\mu = 0.5$, it is sufficient to study the interval $\rho \in [0, 0.5]$. To find a stable phase of the system at a fixed μ , i.e. the phase has a minimum f , we compared three hundred phases of $\rho = i/600$, $i = 1, 2, \dots, 300$.

The classical ground state energy v_0 in Eq. (5), is determined by parameters k , ρ and μ . It has minimums at rational values of ρ . ρ versus μ shows the devil's staircase. The quantum zero point energy f_0 , however, depends only on the parameters k and ρ . The dependence of f_0 on ρ is shown in Fig. 1 for different values of k , where one can see that f_0 takes maximums at rational values of ρ . It has smaller value for incommensurate phases (irrational values of ρ). Furthermore, the positions of the peaks in the figure follow the Farey sequence, i.e., between two peaks at $\rho = p/q$ and $\rho = p'/q'$ there exists a peak at median $\rho = (p+p')/(q+q')$ and it satisfies the condition $\min\{f_0(p/q), f_0(p'/q')\} < f_0[(p+p')/(q+q')] < \max\{f_0(p/q), f_0(p'/q')\}$.

⁽¹⁾In the following, the "quantum effect" simply means the quantum zero point energy effect.

The peaks at high order rationales are indeed flattened. The orders of rationales above which the peaks are flattened are determined by k . And it is found that more and more peaks at rationales of higher orders are flattened as k is increased. The higher the order of the rational, the earlier the peak at the corresponding position is flattened.

The stable phase of the system is a consequence of the competition between the two terms in Eq. (5), v_0 favorites a commensurate phase but f_0 an incommensurate phase. The final phase of the system depends on the parameters \tilde{h} , k , and μ . In the case of $\tilde{h} \ll 1$, i.e., in the classical limit, v_0 gives the major contribution, and it determines the minimum energy phases of the system. Thus the devil's staircase mode-locking in the classical model survive the quantum effect. On the other hand, in the case of relatively large \tilde{h} , the quantum effect dramatically changes the classical mode-locking structure of the system.

In Fig. 2, we plot ρ , at which f has minimum, as a function of μ for different values of \tilde{h} at $k = 1.1$. The thick line in the figure is the result of $\tilde{h} = 0$. The plot shows that those plateaus at $\tilde{h} = 0$ evolve in two different ways as \tilde{h} is increased. Some plateaus at the rationales, whose corresponding peaks in the $f_0 - \rho$ graph is flattened, may persist and even be enhanced in a certain interval as \tilde{h} is increased. For example, in Fig. 1 no peaks show up in the interval $0 < \rho < 1/6$ in curve of $k = 1.1$. However, as \tilde{h} increases, the plateaus at $1/7$, $1/8$, $1/9$ and $1/10$ become more and more evident as is demonstrated in Fig. 2. Similarly, the plateaus at $\rho = 2/11$ and $\rho = 3/17$ expand tremendously as \tilde{h} is increased, while Fig. 1 does not show any peaks at the corresponding positions. The expanding rate of the survived plateaus is different. The plateaus at rationales of higher orders expand faster. On the other hand, the plateaus, at the positions where $f_0 - \rho$ graph shows peaks, are flattened quickly with the increase of \tilde{h} . These plateaus locate at the positions with rationales of lower order. The most interesting result is those new plateaus created at the positions of irrationals. They grow up quickly, and become wide plateaus in the $\rho - \mu$ graph, see e.g., the plateaus designated by the continued fraction representation of the numbers in Fig. 2. These plateaus do not exist at $\tilde{h} = 0$ (thick line).

According to the number theory, a number p/q can be written as a continued fraction

$$\frac{p}{q} = \frac{1}{a_0 + \frac{1}{a_1 + \frac{1}{a_2 \dots}}} \equiv [a_0 a_1 a_2 \dots].$$

A rational is expressed as a finite continued fraction and an irrational a nonterminating continued fraction. For numerical calculation we use the Fibonacci sequence to approach the irrationals, for example we use $\rho = 233/610$ to approximate the golden mean [21111...] and $\rho = 144/521$ the silver mean [31111...][17]. In these cases our computation were performed with 610 and 521 particles, respectively. We call the plateau at an irrational number as '*an irrational plateau*' and refer to this kind of mode-locking as incommensurate phase mode-locking in the following. Surprisingly, the irrational plateau is obviously related to the 'irrationality' of the number (in the sense that the golden mean is the most irrational 'irrational' and then the silver mean and copper mean etc), i.e., the more 'irrational' the number, the easier the system can be locked at. The physical meaning of this statement are two folds. First, by fixing k and increasing \tilde{h} from zero, the first locked irrational plateau appears at the golden mean $\rho = [21111\dots]$ followed by the silver mean $\rho = [31111\dots]$, and then the copper mean $\rho = [4111\dots]$ and so on. The widths of the plateaus are ordered respectively, i.e., for a fixed \tilde{h} , one has $l([21111\dots]) > l([31111\dots]) > l([4111\dots])\dots$, where $l(\rho)$ denotes the width of the plateau at ρ . Second, for a fixed value of k , the number of the irrational plateaus is finite and it increases as k is increased. In the case of $k > 1.5$ most of the mode-locking plateaus seem to be located at the positions of rationals of high order. The only irrational plateau can be recognized is that one locating at the position of the golden mean. With the decrease of k the

irrational plateaus at the silver mean, the copper mean, the iron mean, . . . , and the irrational numbers close to these well-known irrational numbers such as [22111...], [21211...], [32111...] and [31211...] etc. appear gradually. At $k = 1.1$ we find that the plateaus at the silver mean and the copper mean already shown up, as is shown in Fig. 2. Our calculations indicate that at $k = 0.9$ an irrational plateau also appear at the position of the iron mean [51111...]. The irrational plateaus at [61111...], [71111...], and [81111...] show up too at $k = 0.7$, but the plateaus at rationals can not be seen any more when k below this value at relatively large \hbar . This result, i.e. for small k all the rational plateaus are flattened as the quantum effect is increased, agrees with the discovery by Bak and Fukuyama [9] qualitatively.

The mode-locking of the incommensurate phase shown in Fig. 2 has a special meaning to experimentalists. It might allow us to detect the signature of the phase transition by breaking of analyticity[6, 16] in laboratory. The idea is based on the measurement of the specific heat of an incommensurate phase. The specific heat of the system is given by

$$C_v = \sum_{l=1}^N \left(\frac{\omega_l}{T}\right)^2 \frac{e^{\omega_l/T}}{(e^{\omega_l/T} - 1)^2}, \quad (8)$$

where T is the system temperature measured in unit of $\hbar\omega_0/k_B$, and k_B is the Boltzmann constant. C_v is a function of the parameter ρ , k and T . It does not depend on μ . In a commensurate phase e.g. $\rho = 1/3$, we find that C_v decreases exponentially with k . In an incommensurate phase the specific heat shows a quite different behavior. It also decreases exponentially with k for $k > k_c (= 0.9716\dots)$. But it changes insensitively to k for $k < k_c$. This can be easily seen from Fig. 3. Therefore, experimentally when the system is found to be in a locked incommensurate phase, one shall be able to observe this different parameter-dependence behavior in specific heat by changing external parameters such as pressure. This might be useful to verify the existence of k_c in real experiment and detect the manifestation of phase transition by breaking of analyticity.

In summary, we have studied the effect of the quantum zero point energy on commensurate and incommensurate phases. If it is negligible the FK model shows the usual devil's staircase mode-locking, and the system can be locked in commensurate phases at relatively high order. In the opposite case, the scenario changes dramatically and becomes more complex. If k is small the mode-locking plateaus shown up in the classical model are flattened totally by increasing the quantum effect. This result agrees with that of a continuum limit. However, if k is relatively large, the mode-locking plateaus at rationals can be flattened, persistent or even enhanced by the quantum effect. The occurrence of the incommensurate phase mode-locking depends on the degree of irrational of ρ . The mode-locking of incommensurate phase found in this paper provides us a possible way to verify the phase transition by breaking of analyticity experimentally. This phenomenon has not yet been confirmed in laboratory, although it has been predicted theoretically for two decades. We hope that our findings in this paper may draw attentions from experimentalists.

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Fig. 1. – The quantum zero point energy f_0 as a function of ρ . Three different curves correspond to $k = 0.9, 1.1$ and 1.3 , respectively. The peaks happen exactly at rational numbers, while the minimums locate at the irrationals. The number of peaks decreases as k is increased.

Fig. 2. – ρ versus μ . The ρ given in this figure corresponds to that value at which f takes minimum. The curves are ordered from right to left on the left hand side of point P while from right to left on the right hand side of the point as \tilde{h} is increased from 0, 0.05, 0.1, 0.2, 0.3, 0.4.

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Fig. 3. – Specific heat C_v versus k for an incommensurate phase with the golden mean ρ . The temperature is fixed at $T = 0.2$ and $\rho = 233/610$. The curve is obviously divided into two parts. At $k < k_c = 0.9716\dots$ region, C_v is marginally independent of k , while at $k > k_c$ the C_v decreases exponentially.





