Electronic Properties of the 1D Frenkel-Kontorova Model

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The energy spectra and quantum diffusion of an electron in a 1D incommensurate Frenkel-Kontorova model are studied numerically. We found that the spectral and dynamical properties of an electron display quite different behaviors in the invariance circle regime and in the Cantorus regime. In the former case, it is similar to that of the Harper model, whereas in the latter case, it is similar to that of the Fibonacci model. The relationship between spectral and transport properties is discussed.

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The Frenkel-Kontorova (FK) model describes a one-dimensional chain of atoms/particles with harmonic nearest-neighbor interaction placed in a periodic potential. It is a widely used model in condensed matter physics and nonlinear dynamics [1]. For instance, it has been used to model crystal dislocations [2], epitaxial monolayers on the crystal surface [3], ionic conductors and glassy materials [4], an electron in a quasi-1D metal below the Peierls transition [5], charge density waves [6], Josephson junctions chains [7], and dry friction [8]. More recently, this model has been employed to study transport properties of vortices in easy flow channels [9] and strain-mediated interaction of vacancy lines in a pseudomorphic adsorbate system [10]. Because of the competition between the two length scales, the spring length and the period of the on-site potential, the FK model exhibits a wealth of interesting and complex phenomena (see [11] and the references therein).

One of the most striking features of the FK model is the so-called transition by breaking of analyticity. It is shown by Aubry [12] that there exist two different ground state configurations for an incommensurate chain. The transition from one configuration to another occurs when one changes the coupling constant K [see Eq. (2)]. These two incommensurate configurations correspond to invariance circle and Cantorus of the standard map [13], respectively. This transition is still discernible in a quantum FK model [14].

Although extensive studies have been done since its introduction, the FK model continues to attract active interest from different fields. Recent studies are concentrated on phonon modes, because they are responsible for the heat conduction along the chain [15,16]. It is found that the on-site potential breaks the conservation of momentum and makes the heat conduction in the 1D FK model obey the Fourier law [16].

However, the electronic property of the 1D FK model is still unknown up to now. This topic is important from both fundamental and application points of view, because incommensurate and quasiperiodic structures appear in many physical systems such as quasicrystals, two-dimensional electron systems, magnetic superlattices, charge-density waves, organic conductors, and various atomic monolayers absorbed on crystalline substrates. As mentioned before, the FK model has been very successful applied in these systems. It is the purpose of this Letter to study this topic.

The electron in a 1D FK chain obeys the equation

$$t_0(\psi_{n+1} + \psi_{n-1}) + V_n\psi_n = E\psi_n\,, \tag{1}$$

where t_0 is a nearest-neighbor hopping integral which is set to 1 in this Letter, ψ_n is the amplitude of wave function at the nth site, and E is the eigenenergy of electron. The on-site potential, $V_n = \lambda\cos(x_n^0)$, is controlled by parameters λ and x_n^0. $\{x_n^0\}$ is the configuration of an incommensurate ground state of the FK model; namely, $\{x_n^0\}$ minimizes the functional

$$U = \sum_n \frac{1}{2}(x_{n+1} - x_n - a)^2 + K[1 - \cos(x_n)], \tag{2}$$

where K is a coupling constant and a is the equilibrium distance between consecutive atoms. $\{x_n^0\}$ is determined by an adjustable coupling constant K.

In contrast to the Harper model and the Fibonacci model that have been often used to study an electron in incommensurate systems (see review articles [17,18], Ref. [19], and the references therein), the FK model has two control parameters, λ and K, and is thus more general.

Any change in λ and K will alter on-site potential V_n and thus change the electron properties of the system. It is well known that for each irrational number $a/2\pi$ there exists a critical value K_c separating the two configurations of ground state. $K_c = 0.971\,635\,4\ldots$ corresponds to the most irrational number, golden mean value $a/2\pi = (\sqrt{5} - 1)/2$. In this Letter, we restrict ourselves to this particular value in numerical calculations as it is the most used one in the community.

In order to study electron energy spectra, we first obtain ground state configuration for N atoms by the gradient

method [12] for fixed boundaries, i.e., $x_0 \equiv 0$ and $x_N = 2\pi N$. $a/2\pi = (\sqrt{5} - 1)/2$ is approximated by a convergent series of truncated fraction: F_n/F_{n+1} $(n = 1, 2, \ldots)$, where $\{F_n\}$ is a Fibonacci sequence. The number of atoms is chosen as $N = F_n$. The electron eigenenergies are obtained numerically by the transfer matrix method. The transfer matrix $\mathbf{T}_N(E)$ is

$$\mathbf{T}_N(E) = \prod_{n=0}^{N} \mathbf{T}(n, E), \tag{3}$$

where

$$\mathbf{T}(n, E) = \begin{pmatrix} E - \lambda \cos(x_n^0) & -1 \\ 1 & 0 \end{pmatrix}. \tag{4}$$

The allowed energies of an electron satisfy the condition $|\mathrm{Tr}\mathbf{T}_N(E)| \leq 2$. Figure 1 illustrates the spectra as functions of λ for different values of K. From Fig. 1, we can see that for $K \leq K_c$, the energy spectrum (see Fig. 1a) is similar to that of the Harper model, namely, the band splits into subbands as λ is increased from 0. As λ becomes larger than a critical value, energy levels tend to repel each other. There are, however, differences from the Harper model. For instance, the Harper model has a good symmetry, such as self-duality, and the spectrum is symmetric about $E = 0$. All eigenstates are extended when $\lambda < \lambda_c (= 2)$, and localized when $\lambda > \lambda_c$. Our model does not have self-duality and the spectrum is asymmetric. It is known [17] that for a non-self-duality system, there exists a critical parameter above that all eigenstates are localized. Below this critical value, extended, critical, localized states, and mobility edges coexist.

To study the eigenstates quantitatively, the Thouless exponent $[\gamma(E_i)]$ and participation ratios (PR) are calculated for every eigenstate. The Thouless exponent is given by

$$\gamma(E_i) = \int \ln|E_i - E_j| \rho(E_j)\, dE_j = \frac{1}{N} \sum_{j \neq i} \ln|E_i - E_j|, \tag{5}$$

where $\rho(E)$ is the density of states, and the participation ratio is

$$\mathrm{PR} = \frac{(\sum_n \psi_n^2)^2}{N \sum_n \psi_n^4}. \tag{6}$$

The Thouless exponent is proportional to the inverse of the localization length, i.e., $\gamma \sim 1/\xi$. If γ is about the order of $1/N$ for a finite chain of length N, then the eigenstates are extended or critical. Otherwise the eigenstates are localized. In Fig. 2, we plot γ as a function of eigenstate for different λ. Figure 2a is for $K = 0.4$. It tells us that for small λ, all states are extended and critical (correspond to small γ in Fig. 2a). As λ is increased, some eigenstates become localized. For $\lambda > \lambda_c$ all eigenstates are localized. Of course, λ_c depends on K [5]. The minimum Thouless exponent $\gamma_{\min}$ and maximum PR are calculated

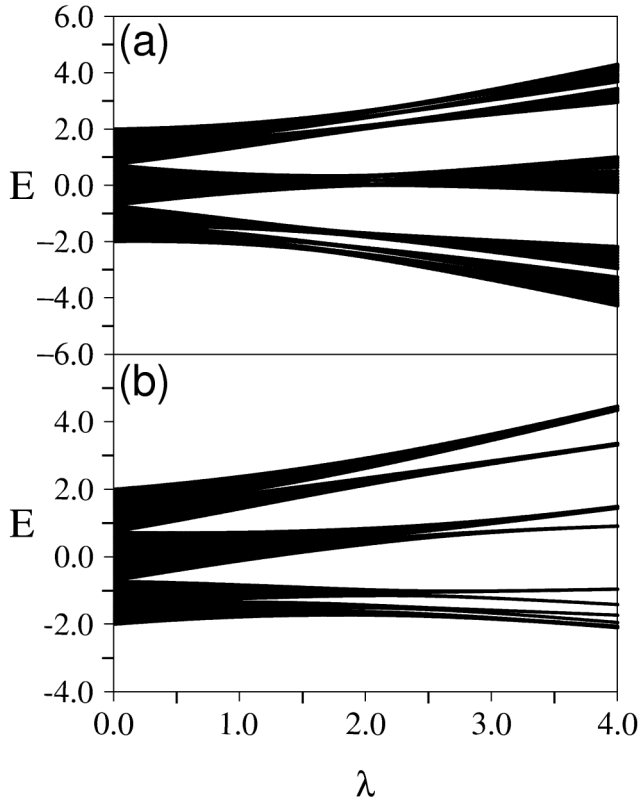

FIG. 1. Energy spectra versus λ for an electron in the FK chains with different values of K. (a) $K = 0.4 < K_c$; (b) $K = 1.6 > K_c$. The chain length is $N = 377$.

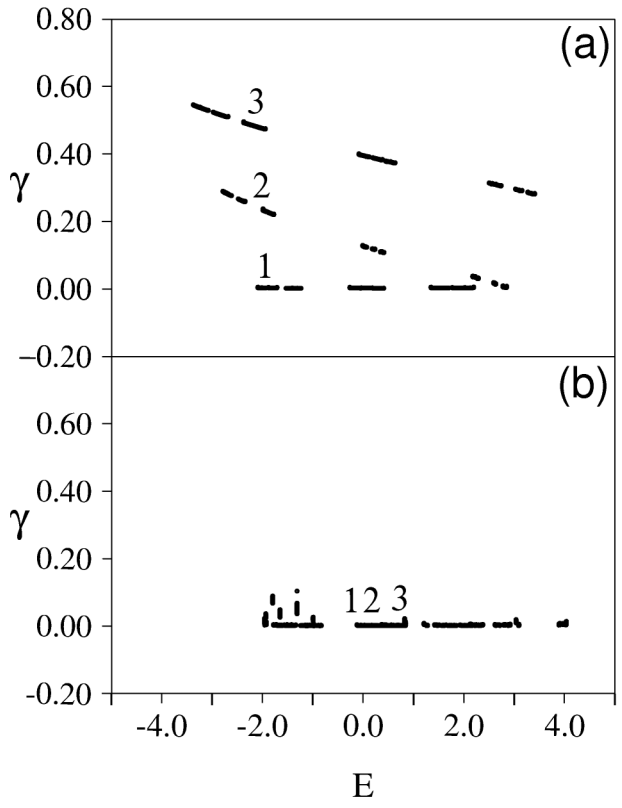

FIG. 2. The Thouless exponent $\gamma(E)$ for different values of K. (a) $K = 0.4$, curves 1, 2, and 3 correspond to $\lambda = 1.0$, 2.3, and 3.0, respectively; (b) $K = 1.6$, curves 1, 2, and 3 correspond to $\lambda = 1.0$, 2.0, and 3.5, respectively. The chain length is $N = 4181$.

as a function of λ so as to find the critical value of λ_c for a fixed K. In Fig. 3, we plot $\gamma_{\min}$ and $\mathrm{PR}_{\max}$ versus λ for $K = 0.4$, 0.6, K_c, and 1.6. From these curves, we can easily obtain critical values $\lambda_c \approx 2.3$, 2.46, and 2.96 for $K = 0.4$, 0.6, and K_c, respectively.

In the case of $K > K_c$, i.e., the ground state configuration of atoms corresponds to Cantorus, both spectra and eigenstates are quite different from that case of $K \leq K_c$ (see Fig. 2b). In this case, no critical value has been found [see curve 4 and curve 2 in Figs. (3a) and (3b), respectively]. All eigenstates are critical. This is similar to that case of quasiperiodic systems such as the Fibonacci chain [19].

To investigate quantum dynamical behaviors, the time evolution of a wave packet in the system described by Eq. (1) is calculated numerically. The wave packet is localized initially at the center of the chain. The time evolution is described by a time-dependent Schrödinger equation

$$i\,\frac{d\psi_n}{dt} = \psi_{n+1} + \psi_{n-1} + \lambda\cos(x_n^0)\psi_n\,. \qquad (7)$$

The variance of the wave packet is

$$\sigma^2(t) = \sum_{n=1}^{N}(n - \bar{n})^2|\psi_n(t)|^2. \qquad (8)$$

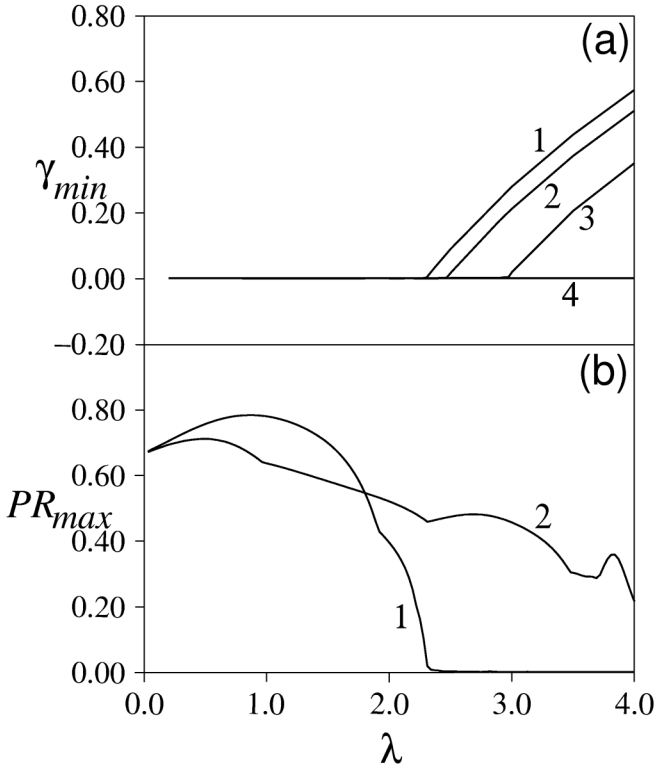

FIG. 3. The minimum Thouless exponent $\gamma_{\min}$ (a) and the maximum participation ratio $\mathrm{PR}_{\max}$ (b) as functions of λ for an electron in the FK chains with different parameter K. Curves 1, 2, 3, and 4 in (a) correspond to $K = 0.4$, 0.6, K_c, and 1.6. Curves 1 and 2 in (b) correspond to $K = 0.4$ and 1.6. The results of $\gamma_{\min}$ and $\mathrm{PR}_{\max}$ are obtained for finite FK chains of length $N = 4181$ and $N = 1597$, respectively.

It can be calculated numerically by integrating the Schrödinger Eq. (7) for a chain of length N with fixed boundaries $\psi_0 = \psi_{N+1} = 0$. In our calculations, the fourth-order Runge-Kutta method with time step $\delta t = 0.01$ was used. The equilibrium ground state positions of N atoms in the FK chain are obtained by the gradient method with the same boundary conditions. The dynamical exponent is defined by $\sigma^2 \sim t^{2\Delta}$.

In Fig. 4, we plot $\sigma^2(t)$ for several values of λ. Figures 4a and 4b correspond to $K = 0.4$ and 1.6, respectively. For $K < K_c$, the time evolution of an electron is also similar to that of the Harper model; that is, $\sigma^2 \sim t^2$ and t^0 for $\lambda < \lambda_c$ ($\lambda = 1.0, 2.2$) and $\lambda > \lambda_c$ ($\lambda = 2.4$), respectively. The unbounded diffusion in the regime of $\lambda < \lambda_c$ is caused by the existence of extended and critical states as discussed above. However, at $\lambda = \lambda_c$, the system displays anomalous diffusion behaviors, and the dynamical exponent depends on K, and $\Delta \approx 1/4$ for $K = 0.4$ (see Fig. 4a). It will be of great interest to connect the exponent of anomalous diffusion with the multifractal dimension of critical eigenstates. For $K > K_c$, the time behaviors of wave packet are similar to that of quasiperiodic systems; i.e., the dynamical exponent Δ depends on λ.

Now we turn to level statistics of the system and its relationship with the dynamical exponent. Geisel *et al.* [20] observed that for a bounded uncountable set of levels, it

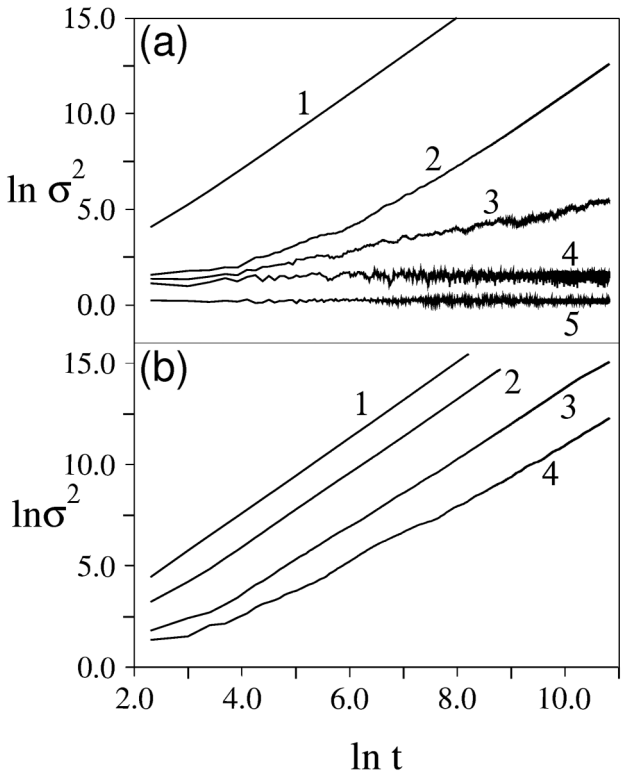

FIG. 4. The variance σ^2 of a wave packet for electrons in the FK chains with different values of K. (a) $K = 0.4$, curves 1, 2, 3, 4, and 5 correspond to $\lambda = 1.0$, 2.2, 2.3, 2.4, and 3.0, respectively, and $\lambda_c \approx 2.3$; (b) $K = 1.6$, curves 1, 2, 3, and 4 correspond to $\lambda = 1.0$, 2.0, 3.0, and 3.5, respectively. The chain length is $N = 10\,946$.

is possible to count the number of energy gaps larger than s and to calculate the integrated level-spacing distribution (ILSD) defined by $p_{\rm int}(s) \equiv \int_s^\infty p(s')\,ds'$. The derivative of the ILSD $p(s) = -dp_{\rm int}/ds$ gives the probability distribution of level spacings. In Fig. 5a we show the ILSD at $\lambda = \lambda_c$ for $K = 0.4$ and 0.6. It can be seen that each distribution consists of two parts: the exponential decay part for small s and the power-law decay part for large s. It is well known that the localization of eigenstates results in the Poisson distribution in energy level spacing statistics [21]. It is thus reasonable to attribute the exponential decay to the localized states, and the power-law-like decay to the critical states, as is the case in the Harper model and the quasiperiodic model. Figure 5b shows the ILSD for several values of λ with $K = 1.6$. Each distribution is very similar to that of the Harper model at λ_c and that of quasiperiodic models. Unfortunately, the power-law-like behavior of the ILDS is not very significant for large λ due to limited bin sizes.

The exponent β for level-spacing distribution defined by $p(s) \sim s^{-\beta}$ can be obtained by the best fit power-law part of ILSD curves. We find that the relation

$$\Delta = 1 - \beta \tag{9}$$

for the Harper model at λ_c is also true for our model in the regime of $K < K_c$, but not for the regime of $K > K_c$.

In summary, we have studied spectral and dynamical properties of an electron in incommensurate FK chains. The system shows a rich phenomenon. For $K < K_c$, i.e., the ground state configuration corresponds to invariance circle, there exists a critical value λ_c above which all eigenstates are localized. Below λ_c, extended, critical, and localized states coexist. The critical value λ_c and dynamical exponent Δ at λ_c depend on K. The relation (9) holds for the power-law part of the ILSD. On the other hand, for the case of $K > K_c$, i.e., the ground state configuration corresponds to Cantorus, all electron eigenstates are critical and Δ depends on λ.

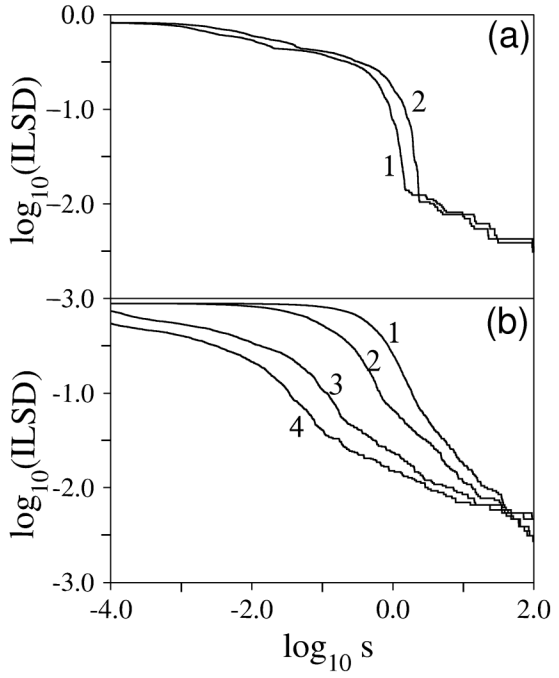

FIG. 5. The integrated level-spacing distribution $p_{\rm int}(s)$ for different values of K. (a) Curve 1 corresponds to $K = 0.4$ and $\lambda_c = 2.3$. Curve 2 corresponds to $K = 0.6$ and $\lambda_c = 2.46$; (b) $K = 1.6$, curves 1, 2, 3, and 4 correspond to $\lambda = 1.0$, 2.0, 3.0, and 3.5, respectively. The chain length is $N = 2584$.

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