Mode entanglement of electrons in the one-dimensional Frenkel-Kontorova model

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We study the mode entanglement in the one-dimensional Frenkel-Kontorova model, and found that quantum entanglement is distinct before and after the transition by breaking of analyticity. We show that the more extended the electron is, the more entangled the corresponding state. Finally, a quantitative relation is given between the average square of the concurrence quantifying the degree of entanglement and the participation ratio characterizing the degree of localization.

Quantum information science has emerged as an active interdisciplinary area between quantum mechanics and information theory [1]. Recently, it was suggested that quantum information science may offer a powerful approach to the study of nonlinear complex quantum systems [2–4]. Specifically, there may be close connections between quantum entanglement theory and many-body theory [1,3]. These ideas motivate us to investigate nonlinear complex quantum systems by entanglement theory.

We investigate quantum entanglement of electrons in the Frenkel-Kontorova (FK) model [5], a paradigm in nonlinear science, and address the effects of the transition by the breaking of analyticity (one striking feature of the FK model) on behaviors of entanglement. The FK model has been used to model various kinds of physical systems such as an electron in a quasi-one-dimensional (1D) metal below the Peierls transition [6]. The FK model describes a 1D chain of atoms with harmonic nearest-neighbor interaction placed in a periodic potential. Due to the competition between the two length scales, the spring length, and the period of the on-site potential, the FK model exhibits a rich complex phenomena [7,8]. It is shown by Aubry [9] that there exist two different ground-state configurations for an incommensurate chain, and the transition from one configuration to another is driven by a single parameter K. These two incommensurate configurations correspond to an invariance circle and cantorus of the standard map [10], respectively.

The electronic properties such as the energy spectrum and quantum diffusion in the FK model have been studied [11]. Quite recently, entanglement properties were studied in the Harper model [12], another paradigm of nonlinear science, and some connections are revealed between entanglement and localization [13]. In contrast to the Harper model that has been often used to study electron properties in incommensurate systems [12,14], the FK model has two control parameters K and λ, which lead to more rich physics. Moreover, the Harper model exhibits a symmetry of self-duality, whereas the FK model does not. Next, we study ground-state entanglement properties of the FK model, and find that the entanglement changes drastically when one goes from one configuration of atoms to another.

Let us start by recalling some basic facts about (spinless) fermions on a lattice of atoms. Consider N local fermionic modes (LFMs)—sites which can be either empty or occupied by an electron [15]. In the second-quantized picture the basic objects are the creation and annihilation operators $c_n^\dagger$ and c_n of nth LFM, satisfying the canonical anticommutation relations $[c_n, c_m]_+ = 0, [c_n, c_m^\dagger]_+ = \delta_{nm}$. The Hilbert space naturally associated with the N LFMs, known as Fock space $\mathcal{H}_F$, is spanned by 2^N basis vectors $|n_1, \ldots, n_N\rangle := \Pi_{l=1}^N (c_l^\dagger)^{n_l}|0\rangle (n_l = 0, 1 \forall l)$.

The fermionic system is indistinguishable and there is no natural tensor product structure, which is essential for the existence of entanglement. However, it is evident that $\mathcal{H}_F$ is isomorphic to the N-qubit space. This is easily seen by defining the mapping [16,17]

$$\Lambda := \prod_{l=1}^N (c_l^\dagger)^{n_l}|0\rangle \mapsto \otimes_{l=1}^N |n_l\rangle = \otimes_{l=1}^N (\sigma_l^+)^{n_l}|0\rangle, \qquad (1)$$

where σ_l^+ is the raising operator of lth qubit. This is a Hilbert-space isomorphism between $\mathcal{H}_F$ and $\mathbb{C}^{\otimes N}$. So, we now have a tensor product structure and the entanglement of fermions can be studied by computing entanglement of qubits.

For a single electron moving on the 1D chain, the general state of the system is given by

$$|\Psi\rangle = \sum_{n=1}^N \psi_n |n\rangle = \sum_{n=1}^N \psi_n c_n^\dagger |0\rangle, \qquad (2)$$

where $|0\rangle$ is the vacuum state. After the mapping, the above state maps to a multiqubit state $\sum_{n=1}^N \psi_n \sigma_n^+|0\rangle$ with only one excitation. This state belongs to the N-dimensional subspace of the whole 2^N-dimensional N-qubit Hilbert space, and the pairwise entanglement quantified by the concurrence [18] is well defined.

Consider an electron hopping in a 1D FK chain described by the following Hamiltonian:

$$H = -t \sum_{n=1}^N (c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) + \sum_{n=1}^N V_n c_n^\dagger c_n, \qquad (3)$$

where t is a nearest-neighbor hopping integral which is set to 1 throughout the paper, and $V_n = \lambda \cos(2\pi\sigma x_n^0)$ is the on-site

potential, which is controlled by the parameter λ and the configuration $\{x_n^0\}$. Here, λ is the amplitude of the on-site potential, $\sigma=F_n/F_{n-1}$ is the inverse distance between two consecutive atoms for $K=0$, and $\{F_n\}$ is a Fibonacci sequence and the series of truncated fraction F_{n-1}/F_n converse to the inverse golden mean $(\sqrt{5}-1)/2$. The number of lattice sites is chosen to be $N=F_n$.

The configuration $\{x_n^0\}$ of the FK model is determined by minimizing the functional

$$U = \sum_n \frac{1}{2}(x_{n+1} - x_n)^2 + K[1 - \cos(2\pi x_n)], \qquad (4)$$

where K is a coupling constant controlling configurations of atoms. Moreover, the periodic boundary condition is assumed for Hamiltonian (3). We can also consider the Heisenberg *XY* model governed by Hamiltonian $H' = -t\Sigma_{n=1}^N(\sigma_n^+\sigma_{n+1}^- + \sigma_n^-\sigma_{n+1}^+)+\Sigma_{n=1}^N\sigma_z$, which describes interaction among N qubits. The *XY* model with one magnon is equivalent to the electronic model with one electron, and all entanglement properties are identical.

From Eqs. (2) and (3), we obtain the eigenequation of the system

$$-t(\psi_{n+1} + \psi_{n-1}) + V_n\psi_n = E\psi_n. \qquad (5)$$

Then, we can obtain the ground state. One-particle ground states are always extended for periodic systems, and can be localized for the FK model as the on-site potential V_n may lead to aperiodicity.

For state (2), the concurrence for two LFMs i and j is easily found to be [19] $C_{ij}=2|\psi_i\psi_j|$. Specifically, when $|\psi_n|=1/\sqrt{N}$, the state becomes the so-called *W* state [20] and the concurrence is given by $2/N$. In this study, we are more interested in the gross measure of entanglement, the average concurrence [13]

$$\langle C \rangle = \frac{1}{M}\sum_{i<j} C_{ij} = \frac{1}{M}\left[\left(\sum_{n=1}^N |\psi_n|\right)^2 - 1\right], \qquad (6)$$

which have connections to localization. Here, $M=N(N-1)/2$. We will mainly concentrate pairwise entanglement of ground states and briefly discuss bipartite entanglement.

As a first step of numerical calculations, we obtain the configuration for N atoms by the gradient method [9], adopting the periodic boundary condition. It is well known that there exists a critical value $K_c=0.154\,641$ separating two configurations of atoms. The configurations determine the on-site potential V_n, and thus ground-state entanglement.

Figure 1 displays behaviors of the average concurrence (6) for the ground state of the FK model as a function of K. When the parameter K increases, we observe an abrupt decrease of the average concurrence near critical value K_c. There is a strong interrelation between the electronic properties and the configurations of atoms, and thus this transition of entanglement results from the transition by breaking of analyticity in configurations of atoms. In other words, the entanglement strongly *feels* the classical transition. For $K<K_c$, the configuration of atoms corresponds to the invari-
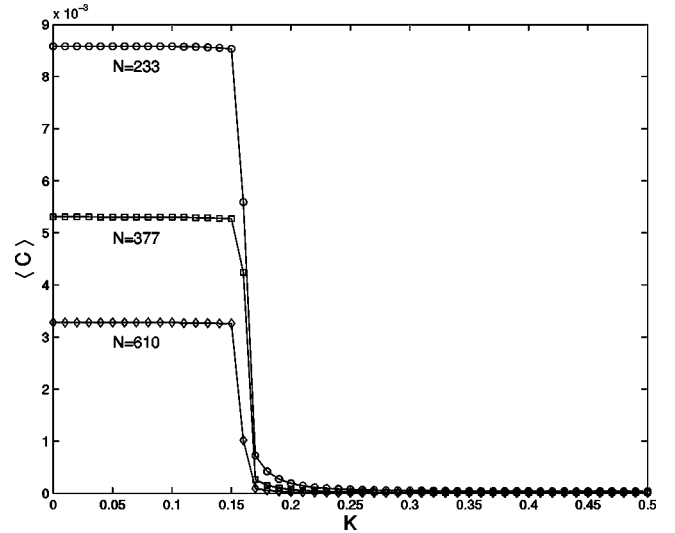

FIG. 1. Average concurrence against parameter K for FK chains with different lengths. The parameter $\lambda=3$.

ance circle. In this case, the concurrences $\langle C \rangle \approx 2/N$ and the ground states are extended. For $K>K_c$, the configuration corresponds to cantorus, and ground states are quite different from the case of $K<K_c$. In this case, the concurrence tends to disappear and the ground state is localized.

To see clearly between the entanglement and localization, we show in Fig. 2 the average concurrence against the participation ratio. The participation ratio characterizing the degree of localization is defined by

$$p = 1 \left/ \left(N\sum_{n=1}^N |\psi_n|^4\right)\right. \qquad (7)$$

We see that the average concurrence increases with the increase of the participation ratio, illustrating that the more
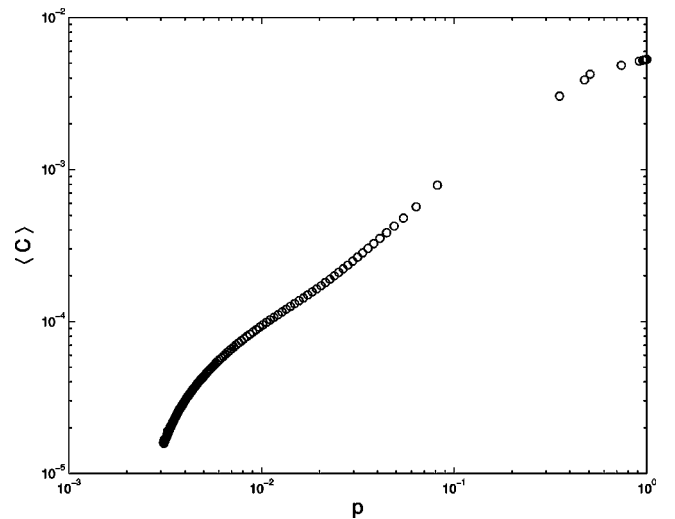

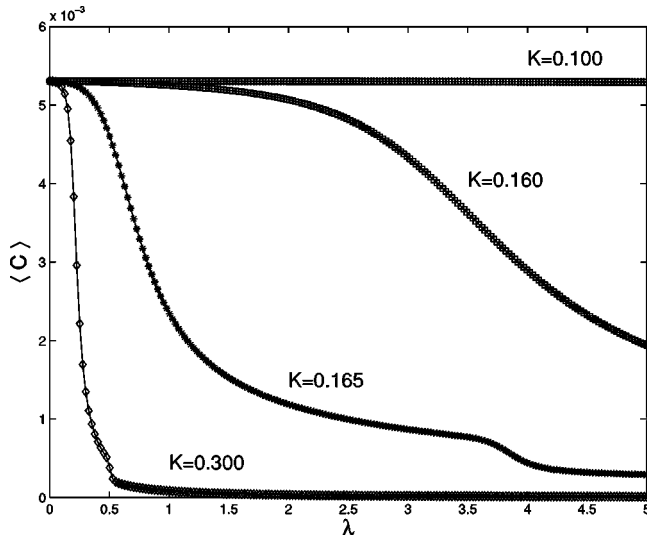FIG. 2. Average concurrence against the participation ratio. The parameters $\lambda=3$ and $N=377$.

FIG. 3. Average concurrence against the parameter λ for different K. The parameter $N=377$.

localized ground states are, the less the average pairwise entanglement.

Now, we investigate effects of amplitude λ of the on-site potential on ground-state entanglement. The average concurrence as a function of λ is shown in Fig. 3 for different K. When $K=0.1$, the concurrence is nearly unchanged, and approximately given by $2/377=0.005305$. As $K<K_c$, atoms are in the configuration before the breaking of analyticity, and this configuration is nearly the same as that for $K=0$. Then, the on-site potential $V_n=\lambda \cos(2\pi\sigma x_n^0)$ are approximately of no difference, and the second term of Eq. (3) contributes a constant to the Hamiltonian for one-particle states. The concurrence of the ground state is then only determined by the first term of Eq. (3), and is thus independent of λ. When $K=0.3$, the concurrence reduces quickly to zero as λ

increases. In this case, the atoms are in the configuration after the breaking of analyticity, and the second term of Eq. (3) no longer commutes with the first one and has significant effects on ground-state properties. For larger λ, the second term dominates over the first one, and thus reduces the entanglement. It is evident that the concurrence goes to zero as $\lambda \to \infty$. The curves for $K=0.16$ and 0.165 display the intermediate behaviors. For $K=0.3$, we observe a critical value λ_c, after which the entanglement tends to zero. The critical value is dependent on parameter K.

So far, we have studied ground-state entanglement properties in the FK model. Next, we investigate dynamics of entanglement with the initial state being $|1\rangle=c_1^\dagger|0\rangle$. Thus, there is no initial entanglement. The time evolution is described by a time-dependent equation ($\hbar=1$)

$$i(d\psi_n)/(dt) = -\psi_{n+1} - \psi_{n-1} + \lambda \cos(2\pi\sigma x_n^0)\psi_n, \qquad (8)$$

which can be integrated numerically by various methods such as the fourth-order Runge-Kutta method.

Figure 4 displays dynamical behaviors of the average concurrence for different K and λ. From Figs. 4(a)–4(c) for $K=0.1$, we observe that the concurrence first linearly increases with time, and finally reaches a plateau, oscillating irregularly around a steady value. The dynamical behaviors only differ slightly for different λ. The reason is similar to that discussed above, namely, for this case the term $\lambda \cos(2\pi\sigma x_n^0)$ contributes a constant to the Hamiltonian and does not alter the system dynamics. In contrast, for $K=0.3$, as seen from Fig. 4(d), the increase of λ suppresses the entanglement generation. When λ becomes larger, the electronic states becomes more localized, and the entanglement diminishes. The slight dependence of λ for $K=0.1$ and the strong dependence of λ for $K=0.3$ corresponds to extended and localized ground states, respectively.
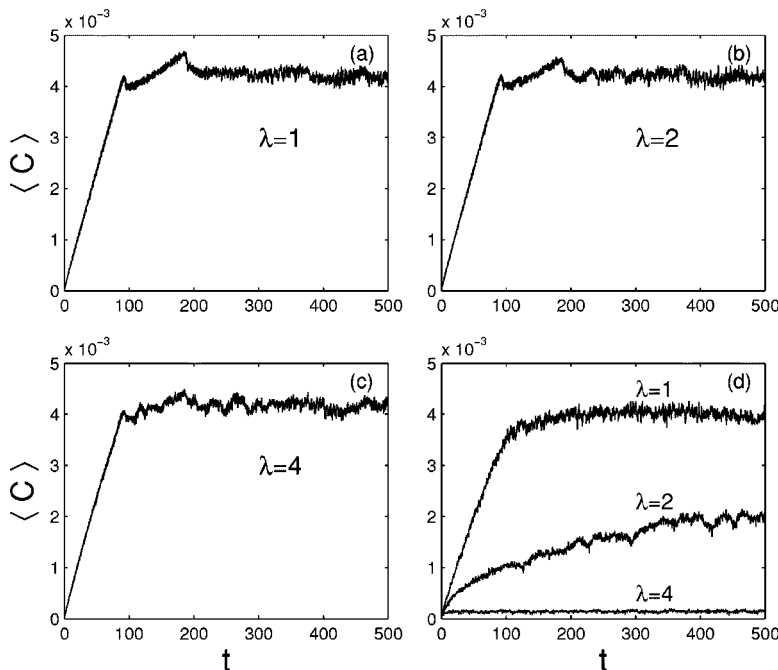

FIG. 4. Time evolution of the average concurrence. The parameter $N=377$. (a), (b), and (c) correspond to $\lambda=1$, $\lambda=2$, and $\lambda=4$, respectively; $K=0.1$. (d) corresponds to $K=0.3$ for different λ. The parameter $N=233$.

From the above results on ground-state and dynamical behaviors of entanglement, we see that the more localized a state is, the less the entanglement. Now, we build a direct quantitative connection between the concurrence, quantifying the pairwise entanglement, and the participation ratio, characterizing the degree of localization. For the one-particle state $|\Psi\rangle$ (2), the concurrence between LFMs i and j $C_{ij} = 2|\psi_i \psi_j|$. We make an average of the square of concurrence, rather than the concurrence,

$$\langle C^2 \rangle = \frac{1}{M} \sum_{i<j} (C_{ij})^2 = \frac{4}{M} \sum_{i<j} |\psi_i|^2 |\psi_j|^2 = \frac{2}{M} \left(1 - \sum_{i=1}^{N} |\psi_i|^4 \right)$$

$$= \frac{4}{N(N-1)} \left(1 - \frac{1}{Np} \right). \quad (9)$$

In deriving the above equation, we have used Eq. (7) and the identity $2\sum_{i<j} |\psi_i|^2 |\psi_j|^2 = 1 - \sum_{i=1}^{N} |\psi_i|^4$, which results from the normalization condition $\sum_{i=1}^{N} |\psi_i|^2 = 1$. Thus, the average of the square of concurrence can be written as a simple function of the participation ratio, and this relation builds a direct connection between pairwise entanglement and localization. It is evident that the larger p is, the larger the concurrence. For the two extreme cases, $p = 1/N$ and $p = 1$, the concurrence C becomes 0 and $4/N^2$, respectively, as we expected. Note that the relation is applicable to arbitrary one-particle states, irrespective of model Hamiltonians.

We have discussed the pairwise entanglement above. For other types of entanglement, such as the bipartite pure-state entanglement quantified by the linear entropy, we also find similar relations as Eq. (9) between the linear entropy and participation ratio [21]. The connections between entanglement and localization are not restricted to electronic systems, and can be applied to other systems such as spin systems with one-magnon excitations. The investigation of multipartite entanglement other than pairwise and bipartite entanglement is more interesting, but at the same time more difficult and complicated.

In conclusion, we have studied ground-state and dynamical pairwise entanglement of two LFMs in the one-dimensional FK model, and found that the entanglement exhibits distinct behaviors for the cases of $K < K_c$ and $K > K_c$. This is a consequence of the transition by breaking of analyticity. For $K < K_c$, the ground state is extended and more entangled; while for $K > K_c$ the ground state is localized and less or not entangled. The amplitude λ of the on-site potential has slight effects on entanglement when $K < K_c$, while it has significant effects when $K > K_c$. It is interesting to note that entanglement is closely connected to localization. It becomes a general feature that the more extended the electron is, the more entangled the electronic state.

Our results support the idea that quantum information theory offers a powerful approach to the study of nonlinear complex system. At the transition point, the concurrence is strongly affected, just as behaviors of the concurrence in the quantum phase transition point [22,23]. It would be more attractive to study entanglement behaviors in other nonlinear complex systems such as two-dimensional quasicrystals and disorder systems.

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