Cantor Spectra for Double Exchange Model

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We numerically study energy spectra and localization properties of the double exchange model at irrational filling factor. To obtain variational ground state, we use a numerical technique in momentum space by “embedded” boundary condition which has no finite size effect a priori. Although the Hamiltonian has translation invariance, the ground state spontaneously exhibits a self-similarity. Scaling and multi-fractal analysis for the wave functions are performed and the scaling indices \( \alpha \)'s are obtained. The energy spectrum is found to be a singular continuous, so-called the Cantor set with zero Lebesgue measure.

The study of the double-exchange (DE) model has a long history. The purposes are to understand the electronic and transport properties of a class of the transition metal oxides, mainly the perovskite manganites, which are known to show the colossal magnetoresistance (CMR). Recent experimental and theoretical studies have revealed that it is a strongly-correlated quantum liquid in which many degrees of freedom are participating, such as orbitals, lattice distortion, electron correlation, dimensionality, the quantum nature of the spin, etc. The current researches are in progress towards the investigation of the systems with many degrees of freedom. A variety of “double-exchange model” have been introduced and investigated from many different viewpoints and approaches.

On the other hand, the minimum model of the DE mechanism has nature still to be clarified even before introduction of the many degrees of freedom. (The model is composed of the itinerant \( e_g \) electron and the localized \( t_{2g} \) spin coupled with the Hund coupling each other.) One is phase separation. They has been found not only in the minimum model also in those with direct exchange couplings between \( t_{2g} \) spins with orbital degree of freedom, and/or with electron correlation. Another is the spin-induced Peierls instability. The ground state is characterized by a charge gap and a modulated spin structure. The charge gap is induced by a commensurate modulation of the transfer integrals. The spin state is distorted with a period commensurate with the Fermi momentum to open the charge gap, thus stabilizing the system. This is isomorphic to the Peierls instability which has been discussed for a long time. The only difference is that the spin degree of freedom is distorted, instead of the lattice degree of freedom.

In this letter, we numerically study the electronic structure of a one dimensional DE model at an irrational filling factor. Although the Hamiltonian has a translation invariance, the energy spectrum spontaneously exhibits a self similarity and forms the Cantor set. The scaling analysis for the band width and the wave functions are performed. We estimate the exponents \( \alpha \)'s which characterize the localization properties. To study the fine structures, usual boundary conditions, such as periodic, twisted or open one, are useless. We use an alternative numerical technique in the momentum space with “embedded” boundary condition. This has no finite size effect a priori. The localization properties and the similarity with the quasi-periodic system are discussed. The electronic and transport properties are found to be completely different from those of the DE model in the literatures.

The DE model we employ is

\[
H = -\left(\sum_{i=1}^{L} t_{i,i+1} c_{i}\dagger c_{i+1} + \sum_{i=1}^{L/2} t_{2i-1,2i+1} c_{2i-1}\dagger c_{2i+1} + h.c.\right) + J \sum_{(i,j)} \vec{S}_i \cdot \vec{S}_j, \tag{1}
\]

where \( c_{i,\sigma} \) is a fermion (\( e_g \) electron) annihilation operator at site \( i \), \( \vec{S}_i \) are localized \( (t_{2g}) \) spins which are treated as classical vectors directed along \( (\theta_i, \phi_i) \) in the spherical coordinates. Moreover, \( J>0 \) is the direct exchange coupling strength between \( t_{2g} \) spins. We fix the parameter to be \( JS^2/t=1 \) throughout this paper. \( L \) (even) is the total number of the sites. The transfer integral \( t_{i,j} \) is given by

\[
t_{i,j} = t \left( \cos \frac{\theta_i}{2} \cos \frac{\theta_j}{2} + e^{-i(\phi_i-\phi_j)} \sin \frac{\theta_i}{2} \sin \frac{\theta_j}{2} \right). \tag{2}
\]

The pure one-dimensional version of the model, i.e. in absence of the second term, all the sub-bands are dispersionless. We introduced the second term only as a perturbation to remove the singular behavior. The singular behavior can be removed by any perturbation and the form of the second term is not special to produce the band width.

We study incommensurate structure as a systematic limit of commensurate ones. The difficulties we meet are the followings: (i) The spin structure of the ground state is expected to be incommensurate, which are very sensitive to
boundary conditions. When we impose periodic, open, or twisted one, the incommensurate structure is restricted to the corresponding space. The true ground state for a finite size does not necessarily exist in the space. (ii) The periodic boundary condition forces to align the spins periodically and spoils the fine structure. One might expect that the incommensurate structure can be asymptotically embedded into the commensurate ones in a sufficiently large system. However, the finite size correction is roughly estimated for $1/L$, which is not small for our purpose. The free boundary condition often induces a boundary state and provides the similar problem. (iii) We need a large denominator of the filling for the scaling analysis. (iv) The ground state has a continuous infinite degeneracy. To be specific, we focus on the cases $\phi_i$ and $\theta_i$. To obtain the ground state, we optimize the functional $E(\{\theta_i, \phi_i\}) = E_{i}(\{\theta_i, \phi_i\}) + JS^2\sum_{\langle ij \rangle} [\cos \theta_i \cos \theta_j + \sin \theta_i \sin \theta_j \cos(\phi_i - \phi_j)]$ by the hybrid use of the conjugate gradient method and the simulated annealing by a monte-carlo method. Here $E_{i}(\{\theta_i, \phi_i\})$ is obtained by the numerical diagonalization of $\mathbf{H}$. We should stress that the infinite system with incommensurate spin structure is embedded into the $2q \times 2q$ matrix in the momentum space without finite size corrections. The numbers of the parameters to be optimized are reduced to $4q$.

Our recursive procedure of arrival to the ground state are the followings: (i) Set $q = 2$. (ii) Under the spin-induced Peierls conjecture, the ground states of $x = p/q$ and $rp/(rq)$ are the same, where $p$, $q$, and $r$ are integers. We optimize the ground state energy for the model with $q$-sites in a unit cell whose lowest $p$ sub-bands are filled. (iii) We optimize the ground state energy for the model with $rq$-sites in a unit cell whose lowest $rp$ sub-bands are filled so that the difference of the energy from (ii) below a desirable precision. (We set here three or four digits.) (iv) Using the same procedure of (iii), we optimize the energy for $p/(rq)$-fillings for each $q$, where $p$ and $q$ are coprimes. Then, we expect that the accuracy is the same that of (iii). (v) Setting $q'$ to be a larger integer than $q$, return to (ii). The procedure (i-v) also provides a cross check of the spin-induced Peierls conjecture. Because this suggests the absence of a more larger modulated structure than $q$-periodic one for $p/q$-filling.

We show the numerical results of the energy spectrum in Fig. 1 where the fillings, $x = p/(2q)$, are exhausted all the combinations of $p = 1, 2, \cdots, 17$ and $q = 1, 2, \cdots, 18$. A Peierls gap, which arose from the spin-induced Peierls mechanism, opens at the Fermi surface. The structure of the energy spectrum is similar to that obtained by Hofstadter [11]. It is observed that the band structures are different between two regions, $x < 0.25$ and $0.25 < x < 0.5$. In the former region, most of the sub-bands have enough dispersion and the energy gaps between the sub-bands are very small. Most of the energy gaps cannot be displayed in this magnification. In the latter, the sub-bands are less dispersive accompanied with larger energy gaps than those of the former.

To see these properties in detail, the electronic properties at the irrational filling are studied as systematic limits of rational ones. To be specific, we focus on the cases $x^{(1)} = \varphi/4$ as a candidate for $x < 0.25$ and $x^{(2)} = \varphi/2$ as that for $0.25 < x < 0.5$, where $\varphi = (\sqrt{5} - 1)/2$. To do this, we use the Fibonacci numbers $F$, defined by $F_{n+1} = F_n + F_{n-1}$ and $F_0 = F_1 = 1$. Then the series of rational number $x^{(j)}_{n} = F_{n-1}/(kF_n)$ converges to $x^{(1)}$ for $k = 4$ and $x^{(2)}$ for $k = 2$ as $n$ becomes large. We denote the number of the sub-bands by $B_n \equiv kF_n (= q)$. In order to specify the branching of the energy bands, we use sequence, $\{c_1, c_2, \cdots\}$ [10].

The energy spectra of the series for $x^{(1)}$ is shown in Fig. 2(a). The energy gaps between the sub-bands are very small. Except for the edge of the spectra, the width of the sub-bands become uniform as the $n$ increases. This suggests that rational $x = p/q$ gives bands with a width varying like $q^{-1}$ for large $q$. The scaling analysis for the width, $W_n$, is shown in the upper part of Fig. 2(a). The states displayed in this figure are (1) the first sub-band just below the
fermi surface, (or edge of the band defined by {0, 1, 1, 1}, ...) and (2) the center of the cluster shown in Fig. 2(a) (or center of the band, {0, 0, 0, 0}). It is observed that \(W_nB_n \sim 1\) (i.e. \(\alpha = 1\)) for (2), while \(W_nB_n \sim 1/B_n\) (i.e. \(\alpha = 1/2\)) for (1). This means that all these states are extended. At the band edge, \(\alpha = 1/2\) when the state is extended. This behavior comes from a remnant of van Hove singularities in 1d bands.

In contrast to those of \(x^{(1)}\), the spectrum for \(x^{(2)}\) forms clusters, as \(n\) increases, accompanied with various size of the energy gaps. (See Fig. 2(b).) The middle part of the spectra for \(n = 5, 6, 7\) and 8 are magnified and shown in the inset. They show a striking similarity with those for \(n = 3, 4, 5\) and 6. This similarity is observed as well in the other regions. (We should note that no self-similarity is found for \(x^{(1)}\). See Fig. 2(a).) The band width at the edges of the clusters seems to go down faster than \(q^{-1}\). The scaling analysis for the width is shown the lower part of Fig. 2(a). The states displays in this figure are the 1st \((\{0, 1, 1, ..., \})\), 2nd, 3rd, and 4th sub-bands from the fermi surface below. For the system with the structure shown in Fig. 2(b), we have to make a extrapolation in \(n\) in every two or three points \(10). W_n is observed to decrease rapidly. The width goes down faster than an algebraic law and is expected to be proportional to \(exp(-\gamma B_n)\) where the \(\gamma\) is a constant. We have \(\alpha = 0\). Thus these states are localized.

The results of the wave function for series for \(x^{(1)}\) and \(x^{(2)}\) are shown in Figs. 3(a) and (b) columns, respectively. They are the wave functions for the energy band just below the fermi surface. For \(x^{(1)}\), the localization length is likely proportional to the \(q\), i.e. number of the sites in a unit cell. The wave function for \(x^{(2)}\) is localized. These properties are consistent with the results from the analysis of the band width. (However, the denominator of the filling is not large enough to make definitive conclusion only from Fig. 3(a).)

We perform the multi-fractal analysis for the wave function. The method was established in \(19, 20\). We use a more developed version \(21\). Extended, critical, and localized states are classified by \(\alpha_{\text{min}} = 1, \neq 1, 0, \text{and} = 0\), respectively. The estimates for the index \(\alpha_{\text{min}}\) is shown in \(21\). It is observed that the \(\alpha_{\text{min}}\) for \(x^{(1)}\) converges to a finite value. This means that the state is not localized. The \(\alpha_{\text{min}}\) for \(x^{(2)}\) is observed to take a small value. This means to the state has a tendency toward localization. These results are consistent with the analysis for the energy spectrum and the behavior of the wave function shown in Fig. 4.

**Discussions:** We have studied the energy spectra and wave function of the DE model at zero temperature. In studies of usual quasi-periodic systems, the quasi-periodicities are introduced by deterministic manners, such as the on-site or off-diagonal quasi-periodicities. In contrast to them, the self-similarity in the DE model is spontaneously obtained from the translation-invariant Hamiltonian \(22\). The modulation of the transfer integral is induced from the spin-induced Peierls instability. In the every step of the iteration toward the irrational filling, the modulation is expressed by \(q\) different amplitudes and, therefore, does not satisfy the Conway’s theorem \(23\). Therefore, the trace map would be described by a transcendental equation.

The numerical results suggest the existence of two, at least, different insulating phases, \(x<0.25\) and \(0.25<x<0.5\). (The scaling analysis of band width, multi-fractal analysis for the wave functions, and the features of the wave function and the energy spectra are mutually consistent.) These phases can be distinguished by dynamical responses, for example, the optical conductivity \(\sigma(\omega)\). Roughly estimated, the optical conductivity is characterized by the the density of states near the Fermi level. The density of states for \(x<0.25\) are very different from those for \(0.25<x\). For \(x<0.25\) the energy gaps between the energy bands are infinitesimally small and the density of states exist except for the Peierls gap. The optical conductivity is approximated by that of a usual band insulator (except for the contribution from the band edges of the subbands). The density of states near the Fermi level. The density of states for \(x<0.25\) are very different from those for \(0.25<x\). For \(x<0.25\) the energy gaps between the energy bands are infinitesimally small and the density of states exist except for the Peierls gap. The optical conductivity is approximated by that of a usual band insulator (except for the contribution from the band edges of the subbands). On the other hand, for \(0.25<x\), the band structure exhibits a self- similarity. In the irrational limit, it is known that the optical conductivity is not well-defined in a usual sense \(22\) and is expected to maintain an anomalous scaling law. (To study the exponents \(24\) it is very interesting. However, even if we use the method proposed in this article the system size and accuracy of the energy are too poor for such an analysis.) The monte-carlo method can be applicable for systems in \(d>1\). In \(d=2\), at any filling \(x\), and for sufficiently large \(J\), it was conjectured \(25\) that the ground state is a flux state whose energy spectrum is similar to the present one. For several fillings \(x\), the conjecture is numerically confirmed \(25\), because the phase factor in the transfer integral can open the Peierls gap \(26\). However, a frustration between the incommensurate structure of the ground state and the periodicity of the periodic lattice arises in \(d=2\). Due to it, to obtain the fine structures of the system are extremely difficult.

The approach in this paper would be one of the fairly good starting points for introducing other degrees of freedom, such as the orbital \(22\), lattice, electron correlation, quantum nature of the spins, anisotropies, etc.

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FIG. 1. Energy spectrum near the Fermi surface as a function of filling \( x \) at \( JS^2/t = 1 \). Spin-induced Peierls gap opens at the fermi surface. We showed half bottom of the full spectrum. For \( x < 0.25 \), the energy bands are divided by small gaps. The gaps are far smaller than the unevenness of carbon print and they look vanishing for the eyes.

FIG. 2. Energy spectra below the fermi surface. (a) Band structures for \( x_n = 1/8 \), 2/12, 3/20, 5/32, 8/52, 13/84, and 21/136 are shown. This series converges to \( x^{(1)} \). Crosses indicate the location of the band edges. The energy gaps between sub-bands are very small. Therefore, the respective crosses which indicate the lower edge of a certain energy band and the upper edge of its lower band look to overlap. (b) Band structures for \( x_n = 2/6 \), 3/10, 5/16, 8/26, 13/42, 21/68, and 34/110 are shown. The series converges to \( x^{(2)} \). The middle clusters for 8/26, 13/42, 21/68, and 34/110 are magnified and shown in the inset.

FIG. 3. (a) Plots of \( W_nB_n \) against \( B_n \) for several states. The upper three are for series \( x^{(1)} \). (Open squares and circles are, respectively, the 1st and 2nd sub-band from the fermi surface below. Crosses are for the band center.) The lower four are for series \( x^{(2)} \). (Bold square, circle, triangle, and rombus are, respectively, the 1st, 2nd, 3rd, and 4th sub-bands from the fermi surface below.) The index of the sequence of the energy bands are \( \{0, 1, 1, 1, 1, \cdots \} \) for the squares and \( \{0, 0, 0, 0, 0, \cdots \} \) for the crosses. (b) Estimates of the scaling index \( \alpha_{\text{min}} \) for \( x^{(1)} \) (open square) and \( x^{(2)} \) (bold square) as a function of \( 1/n \), where \( n \) is the index of \( B_n \).

FIG. 4. The wave functions \( |\psi_i|^{2} \) of the energy band just below the fermi energy, (i.e. \( \{0, 1, 1, 1, \cdots \} \) series), as a function of the site index \( i \). The left and right columns show those for \( x^{(1)} \) and \( x^{(2)} \).
