Unusual metallic phase in a chain of strongly interacting particles

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Abstract

We consider a one-dimensional lattice model with the nearest-neighbor interaction $V_1$ and the next-nearest neighbor interaction $V_2$ with filling factor $1/2$ at zero temperature. The particles are assumed to be spinless fermions or hard-core bosons. Using very simple assumptions we are able to predict the basic structure of the insulator-metal phase diagram for this model. Computations of the flux sensitivity support the main features of the proposed diagram and show that the system maintains metallic properties at arbitrarily large values of $V_1$ and $V_2$ along the line $V_1 - 2V_2 = \gamma J$, where $J$ is the hopping amplitude, and $\gamma \approx 1.2$. We think that close to this line the system is a “weak” metal in a sense that the flux sensitivity decreases with the size of the system not exponentially but as $1/L^\alpha$ with $\alpha > 1$.

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The interest to the theory of one-dimensional systems is only partially related to the study of organic conductors and other quasi-1D compounds. Another source of interest in the 1D physics comes from the variety of problems which are either exactly soluble\textsuperscript{3} or more amenable to computational approach. Their solutions give guidance to intuition which can be applied to problems in higher dimensions.

We consider a 1D system on a lattice with the following Hamiltonian:

\[ H = J \sum_j (a_j^\dagger a_{j+1} + h.c.) + \sum_{i\neq j} V_{|i-j|} n_i n_j \]  

(1)

We study only the filling factor \( \nu = 1/2 \). In the case of the Coulomb potential \( V_{|i-j|} = 1/|i-j| \) one should maintain neutrality and change \( n_i \rightarrow n_i - \nu \).

We consider the spinless fermion system at \( T = 0 \). One can show that for an odd number of electrons \( N \) the Hamiltonian coincides with that for hard-core bosons. For even \( N \) the fermion-boson transformation requires the change of periodic boundary conditions into antiperiodic. The particle-hole symmetry can be shown to require that for even \( N \) at \( \nu = 1/2 \) the states with total quasimomenta \( P, \pi - P, -P, \) and \( P - \pi \) are degenerate.

The system under study undergoes structural and insulator-metal (IM) phase transitions when the hopping amplitude \( J \) is varied. The general point of view is that at small \( J \) the ground state has a crystalline order and is insulating. In the free-fermion limit of large \( J \) the system does not have long-range order and is metallic.

In the case of nearest-neighbor interaction and only then the problem is exactly soluble.\textsuperscript{3,4} In this case the structural transition occurs simultaneously with the IM transition.\textsuperscript{4} In principle, two separate transitions are not forbidden. Nevertheless, in the qualitative arguments below we assume that these transitions are connected to each other and occur at the same \( J_c \).

We concentrate here on the IM transition in a model with the nearest-neighbor and the next-nearest neighbor interactions, the so-called \([V_1, V_2]\)-model. It has been studied\textsuperscript{5} in connection with the spin version of the Hamiltonian Eq. (1). The IM phase diagram for this model has been studied recently in Ref. 6.
We detect the IM transition by analyzing flux sensitivity\(\delta E = |E_p - E_a|\), where \(E_p\) and \(E_a\) are the ground-state energies for periodic and antiperiodic boundary conditions. For simplicity, we take \(E_a\) to be the lowest-energy state with the same quasimomentum \(P\) as \(E_p\).

Starting from the ordered phase at \(J = 0\) and using perturbation theory with respect to \(J\), one can show that \(\delta E \sim J^N\) at small \(J\) and hence falls off exponentially with the system size \(L = 2N\). For free fermions \(\delta E = \pi J/L\). Thus, the dependence of the product \(L\delta E\) on \(L\) and \(J\) is a nice criterion for detection of the IM transition. We obtain this dependence by exact diagonalization technique.

The idea we want to check here is that the IM transition is closely related to the point defect with the lowest energy in the crystalline phase. At finite \(J\) the point defect forms a band. The transition occurs at such \(J\) that the lowest edge of the band comes close to the energy of the ground state. At this point the ground state becomes a strong mixture of the crystalline and defect states. This mechanism reminds the idea of zero-point defectons proposed by Andreev and Lifshitz.

Such a simple picture of the transition implies that the critical value of \(J\) is determined by the energy \(E_d\) of the defect at \(J = 0\). The empirical rule we propose is \(J_c = \beta E_d\), where \(\beta\) is some number. For the exactly soluble problem with nearest-neighbor interaction \(\beta = 0.5\). For the Coulomb problem \(E_d = 2\ln 2 - 1 = 0.386\). Our computations show that for the Coulomb interaction \(J_c\) is between 0.17 and 0.3, which gives \(0.44 < \beta < 0.77\). In the 2D case we have found that \(\beta\) is approximately in the same interval.

Using the empirical relation

\[ J_c = 0.5E_d \]  

we can construct the IM phase diagram for the \([V_1, V_2]\)-model (see Fig. 1). Note that the explicit value of \(\beta\) is not important for the qualitative results. We choose \(\beta = 0.5\) to get the correct value of \(J_c\) for the case \(V_2 = 0\), where it is known exactly. We show below that this is a right choice in a wide range of \(V_1\) and \(V_2\).
Two competing crystalline structures exist in the \([V_1, V_2]-\)model at \(J = 0\). The structure 1 is \(\bullet\circ\circ\circ\), where \(\bullet\) stands for an occupied and \(\circ\) stands for an empty site. The structure 2 is \(\bullet\bullet\circ\circ\).

Dotted lines in Fig. 1 indicate three regions. At \(J = 0\) the structure 1 has the lowest energy in the region I, where \(\Delta \equiv 2V_2 - V_1 < 0\). The lowest-energy defect in this structure has energy \(-\Delta\) and represents a shift of an electron to the nearest site. The structure 2 is stable in the regions II and III, where \(\Delta > 0\). In the region II the lowest defect has energy \(\Delta\) and is also a shift of one electron. In the region III another defect wins, which has energy \(V_2\). This defect is a “domain boundary”, when a portion of a crystal is shifted one site to the right or to the left. Such shift, in fact, produces two domain boundaries simultaneously.

Eq. (2) gives the dependence \(J_c(V_1, V_2)\) that is shown in Fig. 1 with solid lines. These lines separate insulating and metallic phases. To obtain \(J_c(V_1, V_2)\) one should substitute into Eq. (2) the proper expression for the minimum defect energy \(E_d(V_1, V_2)\) at \(J = 0\) in each of three regions as discussed above. The lower solid line shows the IM transition associated with the crystalline structure 1. The upper solid line shows the same transition for the structure 2. It consists of two straight lines in two different regions, II and III, which correspond to the different types of defects.

Fig. 2 shows the results of numerical computation of \(L\delta E/J\) as a function of \(J\) at fixed \(V_1\) and \(V_2\) for a system of 14 electrons. The data for smaller sizes are not shown. However, they have been used to find the critical value \(J_c\) by extrapolation to \(1/L \to 0\). At \((V_1, V_2)\) equal to \((1,0)\), \((0,1)\), and \((1,1)\) our criterion predicts the transition at \(J_c = 0.5\); at \((4,1)\) it predicts \(J_c = 1\). These values are indicated by the points \(a\), \(b\), \(c\), and \(d\) in Fig. 1, and by arrows in Fig. 2. The value \(J_c = 0.5\) is exact for the point \((1,0)\)\(\textsuperscript{3}\). The results of extrapolation give predicted values for the first three points with a 15% accuracy\(\textsuperscript{3}\). For the point \((4,1)\) we have gotten \(J_c = 1.2 \pm 0.1\). Thus, we may conclude that the Eq. (2) works very well in a wide range of \(V_1\) and \(V_2\).

The most important prediction of the phase diagram Fig. 1 is existence of a metallic region between the solid lines which extends infinitely for arbitrarily large \(V_1\) and \(V_2\) close to
the line ∆ = 2V_2 − V_1 = 0. Consider the curves in Fig. 2 corresponding to (V_1, V_2) = (1, 0.48) and (1, 0.52). Now with changing J we are moving almost along the line ∆ = 0 in Fig. 1. In the first case we deviate a little towards the Crystal 1, and in the second case — towards the Crystal 2. Both lines intersect the IM phase lines at large V_1, V_2, predicting J_c = 0.02 in both cases. One can see in Fig. 2 that this prediction is basically fulfilled in the sense that the exponential dependence on J disappears near this point. For J > J_c the system, however, does not look like an ordinary metal, where LδE should be size independent. In fact, we have observed a weak dependence of LδE on L in a wide range of J between J = J_c and J ≈ 0.4.

Fig. 2 also shows δE for (V_1, V_2) = (1, 0.50). Now with decreasing J we are moving exactly along the line ∆ = 0. In this case the exponential transition to the dielectric phase is absent for arbitrarily small J, in agreement with our phase diagram Fig. 1. However, there is some size dependence of LδE along the line ∆ = 0 in the region J ≪ 1. It can be described as δE ∼ 1/L^α with α > 1. Thus, it is not a regular 1D metal where α = 1. An alternative interpretation of the same data would be an exponential size dependence δE ∝ exp(−L/ξ) with anomalously large correlation length ξ.

Now we study more carefully the close vicinity of the line ∆ = 0 far from the origin. In the region ∆ ≪ V_1, V_2 the spectrum of energies at J = 0 has two scales. The large scale is determined by V_1 and V_2, while the second scale is |∆|, which is the energy necessary to produce a defect. When ∆ = J = 0 the ground state is macroscopically degenerate.

To separate these two scales we consider a limit V_1, V_2 → ∞, J and ∆ being finite. In this limit the size of the Hilbert space can be greatly reduced. Only the states which are degenerate at ∆ = J = 0 should be taken into account. These states are such that neither three electrons nor three holes occupy adjacent sites.

The reduction of the Hilbert space size is from C_L^{L/2} to approximately f_{L−2}, where f_n denote the Fibonacci numbers, defined by f_n = f_{n−1} + f_{n−2}, f_0 = f_1 = 1. At large n one has f_n ≈ ((1 + √5)/2)^n+1/√5.

With this reduction we can increase L up to 40 (f_{38} = .63 × 10^8). Fig. 3 shows LδE/J as
a function of $\Delta/2J$ obtained for different $L$. The maximum occurs not at $\Delta = 0$, as can be expected from naive consideration, but at $\Delta/2J \approx -0.6$. Accurate size extrapolation shown in Fig. 4 demonstrate that at this point $\delta EL/J$ stays finite as $L$ goes to infinity. Thus, the system at $\Delta \approx 1.2J$ is a normal metal. The flux sensitivity in the limit $L \to \infty$ is less than the value $\pi$ for free fermions and is equal $L\delta E/J \approx 2.5$. In the phase diagram Fig. 1 the “magic” metallic line $\Delta = 1.2J$ is shown with dashed line. This line appears, obviously, as a result of quantum mixture of the two different ordered phases.

Fig. 3 shows also the energy per particle as a function of $\Delta/2J$ obtained in the same limit. We have not found any singularity in the energy in the region of interest. The gap between the ground and the lowest excited states with the same total quasimomentum at the magic metallic line scales to zero linearly in $1/L$, as shown in the inset to Fig. 3. Note that usually a crystalline phase on the lattice has a finite gap.

The inset in Fig. 4 shows the reciprocal correlation length $1/\xi = -d\ln(L\delta E)/dL$ as a function of $\Delta/2J$ as obtained from the slopes of the curves in Fig. 4 at largest $L$. Note that the condition $\xi < L$ corresponds to $1/\xi > 0.25$. Thus, we have a real exponential behavior for $-3 < \Delta/2J < 2$. At large negative values of $\Delta/2J$ the ground state of the system is the crystal with the structure 2 with a small admixture of defects which are fragments of the structure 1. At large and positive $\Delta/2J$ one has the opposite picture. In the intermediate region the ground state is a mixture of these two structures. If we extrapolate $1/\xi$ in each of the exponential regions, we find that it turns into zero approximately at the boundaries of the metallic strip, shown by two parallel solid lines in Fig. 1. This is natural, since the naive picture which leads to Fig. 1 does not take into account mixing of two crystalline structures.

The small value of $\xi$ in the intermediate region suggests that the size dependence of $L\delta E$ is not exponential near the magic line. This would imply the existence of another phase, which may be named a “weak metal.” If such phase exists, there should be a phase lines which separate the weak metal from the normal metal, where $L\delta E$ is size independent. The inset in Fig. 1 shows schematically the region of the normal metallic phase. This diagram is similar to the one obtained in Ref. 6, except it predicts an infinite metallic line in the plane.
Finally, we have shown that a simple rule Eq. (2) provides a reasonable description of the phase diagram of IM transition in the \([V_1, V_2]\)-model. We have found an interesting metallic phase which exists at any small values of \(J\). The ground state of this phase is a mixture of two crystalline phases with moving boundaries. The nature of a small deviation of the metallic phase from the line \(\Delta = 0\) is not clear.

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FIGURES

FIG. 1. Phase diagram of \([V_1, V_2]\)-model. Solid lines show the diagram as obtained from Eq. (2). The dotted lines separate regions I, II, and III. The point \(a\) is known exactly; the points \(b, c,\) and \(d\) are checked by computations. The long-dashed lines in the main figure and in the inset show the “magic” metallic line. The short-dashed lines in the inset show schematically the region of the normal metallic phase where \(L\delta E\) independent of \(L\).

FIG. 2. Dependence of flux sensitivity in units of \(J/L\) on \(J\) for different \((V_1, V_2)\) for the system with 14 electrons as obtained by exact diagonalization. The arrows show the transition points predicted by the phase diagram. The dashed line shows the free fermion result \(L\delta E/J = \pi\).

FIG. 3. Flux sensitivity \(L\delta E/J\) for different \(L\) and the ground-state energy \(E\) per particle for \(L = 40\) as functions of \(\Delta/2J\). The energy \(E\) is measured from the classical energy of the crystalline structure 2. The inset shows the excitation gap along the magic metallic line vs. \(1/L\). All results are obtained by exact diagonalization in the limit \(V_1, V_2 \to \infty\).

FIG. 4. Size dependence of flux sensitivity for different values of \(\Delta/2J\) in the limit \(V_1, V_2 \to \infty\). The inset shows the slope \(1/\xi\) as obtained from this size dependence at large \(L\) vs. \(\Delta/2J\). The slope \(1/\xi\) can be considered as the reciprocal correlation length when \(\xi < L \sim 40\).
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12 See Ref. 11.

13 We claim such a high accuracy for the result of extrapolation because the size dependence looks very similar to the case $(V_1, V_2)=(1,0)$, where exact $J_c$ is known. In the Coulomb case the extrapolation is more uncertain.

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E.V. Tsiper and A.L. Efros, Unusual Metallic Phase..., Fig. 1
[E.V. Tsiper and A.L. Efros, Unusual Metallic Phase..., Fig. 2]
$\frac{E}{JN}$,
$L = 40$

$\frac{\Delta}{2J}$

Gap

$\frac{1}{L}$ 0.1
\( (L/J) \delta E \) vs. \( \Delta/2J \) for different values of \( \xi/L \).