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LETTER TO THE EDITOR

An 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-neighbour interaction V_1 and the next-nearest-neighbour 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 the sense that the flux sensitivity decreases with the size of the system not exponentially but as $1/L^\alpha$ with $\alpha > 1$.

The interest of 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 is the variety of problems which are either exactly soluble [1] or more amenable to a 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:

$$H = J \sum_j (a_j^\dagger a_{j+1} + \text{HC}) + \sum_{i \neq j} V_{|i-j|} n_i n_j. \tag{1}$$

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 make the change $n_i \to n_i - \nu$.

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 ones. 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-neighbour interaction, and only then, the problem is exactly soluble [2–4]. In this case the structural transition occurs simultaneously with the IM transition [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.

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We concentrate here on the IM transition in a model with nearest-neighbour and next-nearest-neighbour interactions, the so-called $[V_1, V_2]$ model. It has been studied [5] in connection with the spin version of the Hamiltonian, equation (1). The IM phase diagram for this model has been studied recently in reference [6].

We detect the IM transition by analysing the flux sensitivity [7, 8] $\delta E = |E_p - E_a|$, 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 the exact-diagonalization technique.

The idea that 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 [9]. At this point the ground state becomes a strong mixture of the crystalline and defect states. This mechanism reminds us of the idea of zero-point defectons proposed by Andreev and Lifshitz [10].

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 that we propose is $J_c = \beta E_d$, where β is some number. For the exactly soluble problem with nearest-neighbour interaction, $\beta = 0.5$. For the Coulomb problem, $E_d = 2\ln 2 - 1 = 0.386$. Our computations [11] 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 β is approximately in the same interval.

Using the empirical relation

$$J_c = 0.5E_d \tag{2}$$

we can construct the IM phase diagram for the $[V_1, V_2]$ model (see figure 1). Note that the explicit value of β is not important for the qualitative results. We choose $\beta = 0.5$ to get the correct value of J_c for the case where $V_2 = 0$, where it is known exactly. We show below that this is the right choice for 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 $\bullet\circ\bullet\circ$, where $\bullet$ stands for an occupied site and $\circ$ stands for an empty site. The structure 2 is $\bullet\bullet\circ\circ$.

Dotted lines in figure 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 Δ 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 a shift, in fact, produces two domain boundaries simultaneously.

Equation (2) gives the dependence $J_c(V_1, V_2)$ that is shown in figure 1 with solid lines. These lines separate insulating and metallic phases. To obtain $J_c(V_1, V_2)$ one should substitute into equation (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

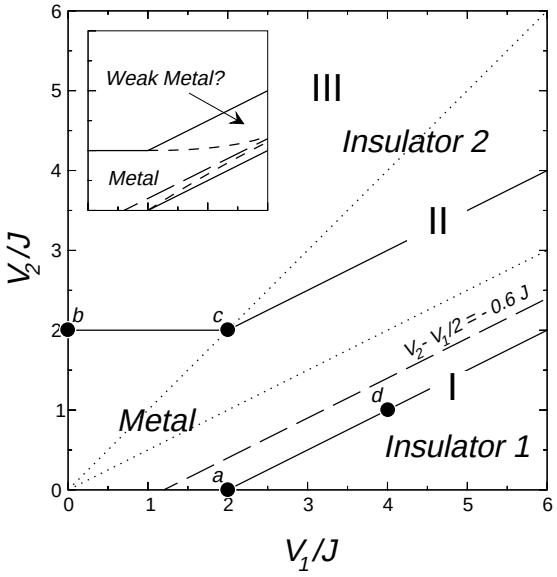

Figure 1. The phase diagram of the $[V_1, V_2]$ model. Solid lines show the diagram as obtained from equation (2). The dotted lines separate regions I, II, and III. The point a is known exactly; the points b, c, and d are checked by computations. The long-dashed lines in the main figure and in the inset 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.

III, which correspond to the different types of defect.

Figure 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 $1/L \to 0$. For (V_1, V_2) equal to (1, 0), (0, 1), and (1, 1), our criterion predicts the transition at $J_c = 0.5$; for (4, 1) it predicts $J_c = 1$. These values are indicated by the points a, b, c, and d in figure 1, and by arrows in figure 2. The value $J_c = 0.5$ is exact for the point (1, 0) [2–4]. The results of extrapolation give predicted values for the first three points with a 15% accuracy [12]. For the point (4, 1) we got $J_c = 1.2 \pm 0.1$. Thus, we may conclude that equation (2) works very well over a wide range of V_1 and V_2.

The most important prediction of the phase diagram given as figure 1 is the existence of a metallic region between the solid lines which extends infinitely for arbitrarily large V_1 and V_2 close to the line $\Delta = 2V_2 - V_1 = 0$. Consider the curves in figure 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 $\Delta = 0$ in figure 1. In the first case we deviate a little towards crystal 1, and in the second case we deviate a little towards 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 figure 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 $L\,\delta E$ should be size independent. In fact, we have observed a weak dependence of $L\,\delta E$ on L over a wide range of J between $J = J_c$ and $J \approx 0.4$.

Figure 2 also shows δE for $(V_1, V_2) = (1, 0.50)$. Now with decreasing J we are moving exactly along the line $\Delta = 0$. In this case the exponential transition to the dielectric phase is absent for arbitrarily small J, in agreement with our phase diagram, figure 1. However,

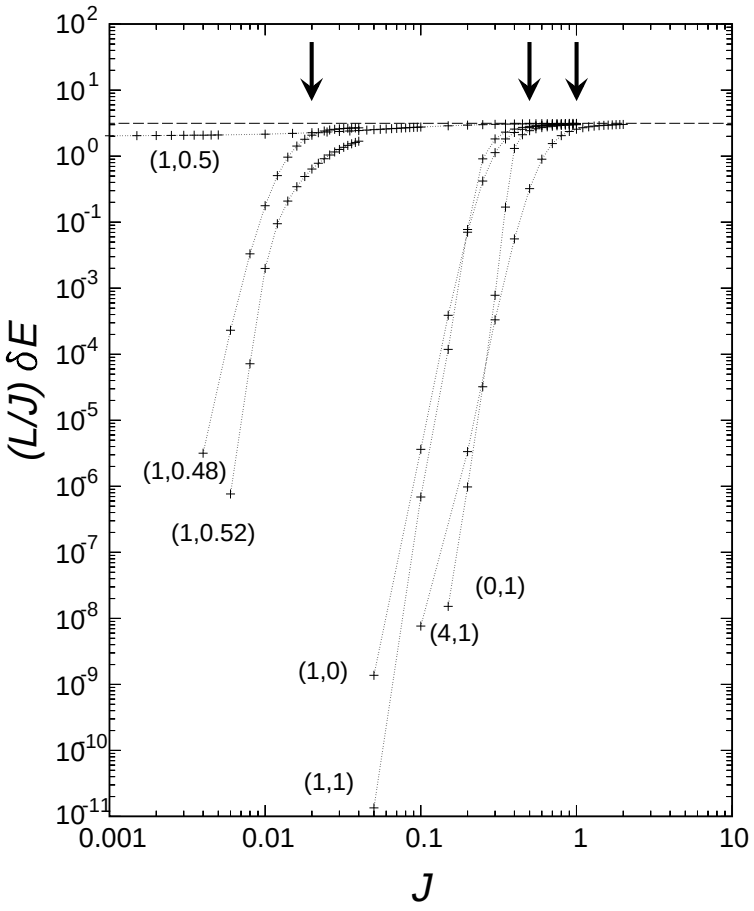

Figure 2. The dependence of the flux sensitivity in units of J/L on J for different (V_1, V_2) for the system with 14 electrons as obtained by exact diagonalization. The arrows show the transition points predicted by the phase diagram. The dashed line shows the free-fermion result $L\,\delta E/J = \pi$.

there is some size dependence of $L\,\delta E$ along the line $\Delta = 0$ in the region $J \ll 1$. It can be described as $\delta E \sim 1/L^{\alpha}$ with $\alpha > 1$. Thus, this is not a case of a normal 1D metal where $\alpha = 1$. An alternative interpretation of the same data would be an exponential size dependence, $\delta E \propto \exp(-L/\xi)$, with an anomalously large correlation length ξ.

Now we study more carefully the immediate vicinity of the line $\Delta = 0$ far from the origin. In the region $\Delta \ll V_1, V_2$, 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 $|\Delta|$, which is the energy necessary to produce a defect. When $\Delta = J = 0$, the ground state is macroscopically degenerate.

To separate these two scales we consider a limit $V_1, V_2 \to \infty$, J and Δ being finite. In this limit the size of the Hilbert space can be greatly reduced. Only the states which are degenerate at $\Delta = J = 0$ 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 the

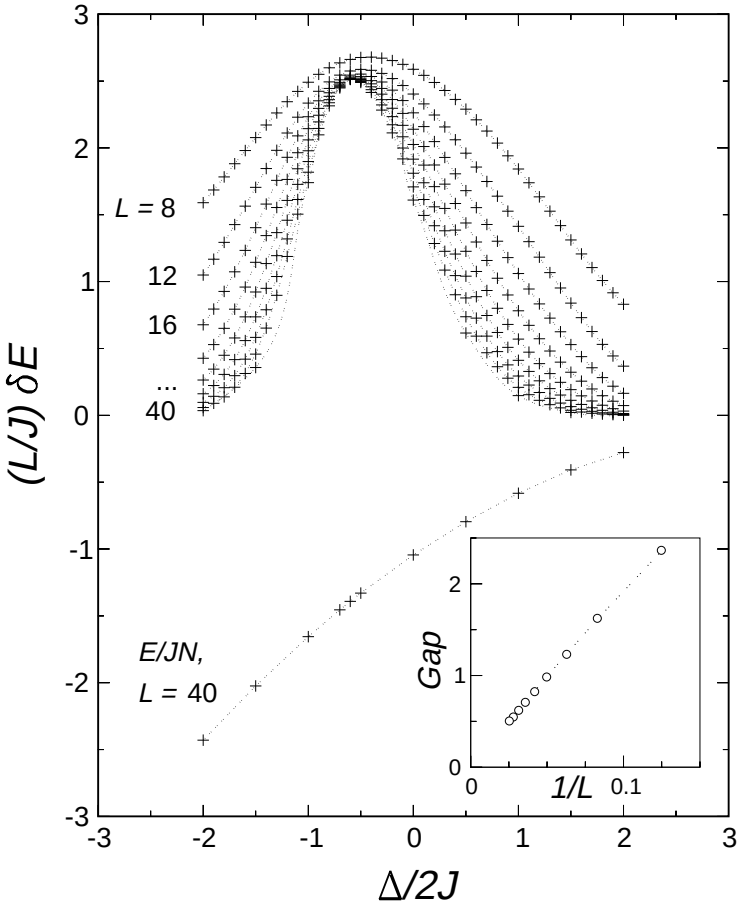

Figure 3. The flux sensitivity $L\,\delta E/J$ for different L and the ground-state energy E per particle for $L = 40$ as functions of $\Delta/2J$. The energy E is measured from the classical energy of the crystalline structure 2. The inset shows the excitation gap along the magic metallic line versus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

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 [13] $f_n \approx ((1+\sqrt{5})/2)^{n+1}/\sqrt{5}$.

With this reduction we can increase L up to 40 ($f_{38} = 0.63 \times 10^8$). Figure 3 shows $L\,\delta E/J$ as a function of $\Delta/2J$ obtained for different L. The maximum occurs not at $\Delta = 0$, as could be expected from naive consideration, but at $\Delta/2J \approx -0.6$. The accurate size extrapolation shown in figure 4 demonstrates that at this point $\delta E\,L/J$ 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 π for free fermions and is equal to $L\,\delta E/J \approx 2.5$. In the phase diagram, figure 1, the 'magic' metallic line $\Delta = 1.2J$ is shown as a dashed line. This line appears, obviously, as a result of a quantum mixture of the two differently ordered phases.

Figure 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

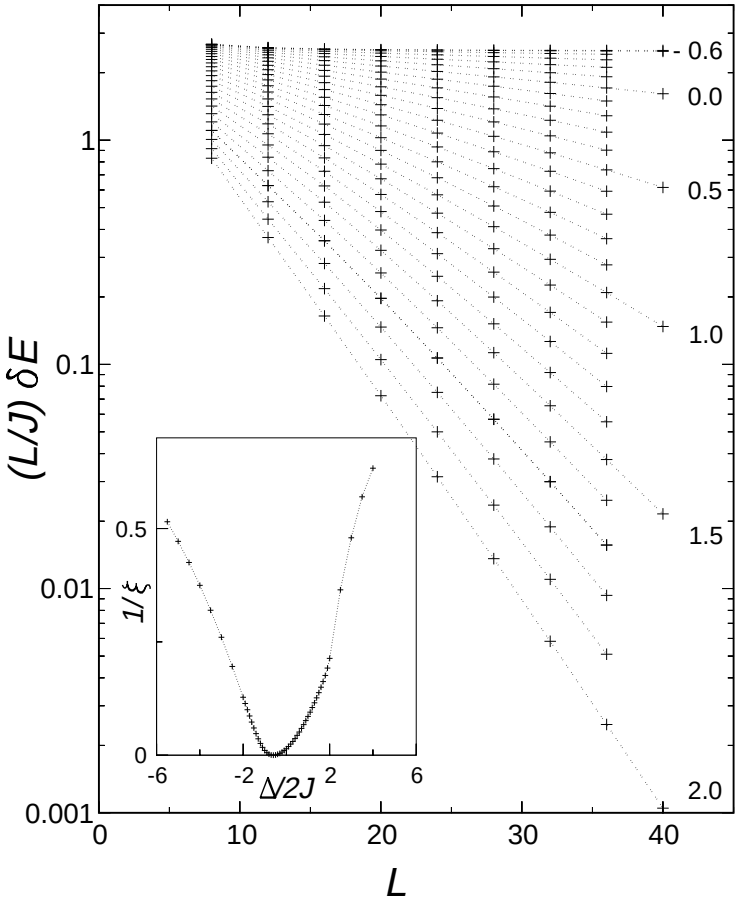

Figure 4. The size dependence of the flux sensitivity for different values of $\Delta/2J$ in the limit $V_1, V_2 \to \infty$. The inset shows the slope $1/\xi$ as obtained from this size dependence at large L versus $\Delta/2J$. The slope $1/\xi$ can be considered as the reciprocal correlation length when $\xi < L \sim 40$.

magic metallic line scales to zero linearly in $1/L$, as shown in the inset to figure 3. Note that usually a crystalline phase on the lattice has a finite gap.

The inset in figure 4 shows the reciprocal correlation length $1/\xi = -\mathrm{d}\ln(L\,\delta E)/\mathrm{d}L$ as a function of $\Delta/2J$ as obtained from the slopes of the curves in figure 4 at the largest L. Note that the condition $\xi < L$ corresponds to $1/\xi > 0.25$. Thus, we have a real exponential behaviour 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 becomes zero approximately at the boundaries of the metallic strip, shown by two parallel solid lines in figure 1. This is natural, since the naive picture which leads to figure 1 does not take into account mixing of two crystalline structures.

The small value of ξ 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 a phase exists, there should be phase lines which separate the weak metal from the normal metal, where $L\,\delta E$ is size independent. The inset in figure 1 shows schematically the region of the normal-metallic phase. This diagram is similar to the one obtained in reference [6], except that it predicts an infinite metallic line in the plane (V_1, V_2).

Finally, we have shown that a simple rule, equation (2), provides a reasonable description of the phase diagram of the IM transition in the $[V_1, V_2]$ model. We have found an interesting metallic phase which exists at any small value 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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This result clearly contradicts the statement made by Poilblanc *et al* in reference [6] that a 1D Coulomb system is metallic for all J.
[12] We claim such a high accuracy for the result of the extrapolation because the size dependence looks very similar to that in the case where $(V_1, V_2) = (1, 0)$, where an exact value of J_c is known. In the Coulomb case the extrapolation is more uncertain.
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