Mott transition in quasi-one-dimensional systems

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We report the application of the density-matrix renormalization-group method to a spatially anisotropic two-dimensional Hubbard model at half filling. We find a deconfinement transition induced by the transverse hopping parameter t_y from an insulator to a metal. Therefore, if t_y is fixed in the metallic phase, increasing the interaction U leads to a metal-to-insulator transition at a finite critical U. This is in contrast to the weak-coupling Hartree-Fock theory which predicts a nesting-induced antiferromagnetic insulator for any $U > 0$.

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The metal-insulator transition (MIT), also called the Mott transition,[1] is certainly one of the most difficult challenges facing condensed-matter theorists. Hubbard,[2] in a pioneering work, introduced a simple one-band Hamiltonian which has only two parameters: t for the kinetic energy of the electrons and U for the local electron-electron interactions. This model is at half filling the model of reference for the MIT. In $D = 1$, Lieb and Wu[3] obtained an exact solution by using the Bethe ansatz. The ground state is an insulator for any $U/W > 0$, where W is the bandwidth. Thus, the MIT occurs at the critical value $(U/W)_c = 0$. In infinite dimensions, the dynamical mean-field theory (DMFT)[4,5] predicts a critical point at $(U/W)_c \approx 1$.

The discovery of layered materials, where the motion of electrons driving the low-energy physics is mostly confined in the layers, has raised great interest in the two-dimensional (2D) Hubbard model. The physics at large $U/W \gtrsim 1$ is now understood, the charge excitations are gapped, and the spin excitations are described by the Heisenberg Hamiltonian which has long-range order (LRO) at $T = 0$. But for $U/W \lesssim 1$, the physics is still unclear. Our current knowledge about the weak-coupling regime is mostly drawn from the Hartree-Fock approximation and from quantum Monte Carlo (QMC) simulations.[6,7] The QMC results agree qualitatively with the Hartree-Fock prediction that the ground state is a Slater insulator for any $U/W > 0$. However, in most recent studies, such as in Ref. 7, even though considerable progress has been achieved in reaching larger systems, in the weak U regime where the eventual gap is small, reliable extrapolations of the QMC data remain difficult to achieve. It would thus be preferable to apply finite-size scaling for data analysis instead of relying on extrapolations.

More recently, extensions of the DMFT which include nonlocal fluctuations, the dynamical cluster approximation (DCA),[8] or the cellular DMFT,[9,10] have been applied to the 2D Hubbard model. The focus in these studies has mostly been to discuss the nature of the MIT within the paramagnetic solution of the DMFT equations. A systematic comparison of the possible ordered or disordered ground states as functions of the cluster sizes is still lacking. Therefore, the issue as to whether or not quantum fluctuations destroy the Hartree-Fock solution in the half-filled 2D Hubbard model in the small U regime remains open.

In this paper, we show that insight into this problem can be gained by studying the quasi-1D Hubbard model. We apply the two-step density-matrix renormalization group (DMRG)[11] to an array of coupled Hubbard chains. We find that there is a deconfinement transition from the 1D insulator toward a metallic phase as the transverse hopping t_y is increased from 0. Hence, for a fixed t_y in the metallic phase, there is a quantum phase transition (QPT) at a finite quantum critical point (QCP) $(U/W)_c$. This suggests, as seen in the limit of infinite dimensions,[4] that by freezing out the local time dynamics, the Hartree-Fock approximation is unable to account for the physics of the Hubbard model even for weak interactions. We note that Biermann and co-workers[12] applied the chain-DMFT to the quasi-1D Hubbard model. They also found a deconfinement transition. However, they were restricted to paramagnetic solutions. Hence, unlike our study, they could not tell whether or not their metallic solution is the true ground state of the quasi-1D Hubbard model. A deconfinement transition was also predicted by Essler and Tsvelik[13] in a related model with a long-ranged transverse hopping.

Let us briefly describe the two-step DMRG method introduced for coupled chains in Ref. 11. This method is generalized here for coupled multileg ladders. For a system of spins or electrons on an anisotropic square lattice of dimensions $L_x \times L_y$, the Hamiltonian may be written as $H = H_{\text{intra}} + H_{\text{inter}} = \sum_l h_l + g\tilde{H}_{\text{inter}}$, where h_l are the Hamiltonians of 1D systems; $g \ll 1$ is the transverse coupling. $\tilde{H}_{\text{inter}}$ is of the same magnitude as H_{intra}. h_l can represent a single chain, a two-leg ladder, or even a multileg ladder as illustrated in Fig. 1 for a spin system. The DMRG analysis of H is done in two steps. In the first step, the m_2 lowest eigenfunctions ϕ_n and eigenvalues E_n from different charge-spin sectors of the 1D Hamiltonian h_l are obtained by applying the conventional 1D DMRG algorithm.[14] During this step, m_1 states are kept such that the lowest m_2 states are accurately computed. In the second step, H is projected onto the tensor product of the ϕ_n's. Since the resulting effective 2D Hamiltonian is now 1D in the transverse direction, it can be studied using the conventional DMRG. For a given size, let E_0 and E_{m_2} be the lowest and the highest DMRG energies kept for h_l. If $g \ll \Delta E = E_{m_2} - E_0$ (in practice we set $\frac{g}{\Delta E} \simeq 10$), the two-step DMRG retains high accuracy. But as L_x increases, ΔE decreases, for a fixed g, it would be impossible to retain accuracy for arbitrarily large L_x. Thus, successfully performing finite-size analysis for the g-induced QPT will depend on the magnitude of the critical value of g and on the density of the 1D spectrum.

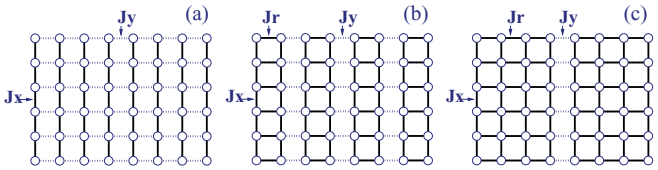

FIG. 1. (Color online) Clusters used as building blocks for the 2D square lattice: (a) chains; (b) two-leg ladders; and (c) four-leg ladders: $J_x = 1$ is the coupling along the legs; J_y is the intercluster coupling, and J_r is the coupling between the rungs for the ladders.

In order to avoid uncertainties related to extrapolations in the regime where the gap is very small, it is preferable to perform finite-size scaling analysis. In the vicinity of the QCP the gap is $\Delta(g) \propto (g_c - g)^{\nu}$, where ν is the correlation length exponent (Lorentz invariance is assumed), and g_c is the value of the g at the QCP. The product $L\Delta$, where L is the linear size of the system, is given by a universal function, $L\Delta = f[C(g_c - g)L^{1/\nu}]$,[15] where C is independent of L. At the critical point, $L\Delta = f(0)$ is independent of L. All the curves $\Delta(g)$ for different sizes should converge at $g = g_c$. In practice, however, there are finite-size effects. It is necessary to extrapolate the different crossing points in order to precisely locate g_c. Before studying the MIT in the Hubbard model, we first apply the two-step technique to the QPT in quantum antiferromagnets (AFM). There are two motivations for this prelude on spin systems. First, well-controlled QMC are available; this will allow one to gauge the performance of the two-step DMRG. Second, the energy scales of the different systems roughly span those of the Hubbard model when the interaction is varied.

In coupled chains with $S = 1$, the ground state is known both in 1D and 2D. In 1D, the system has a spin gap, the Haldane gap $\Delta_{S=1} = 0.410\,49$,[16] The correlation length is $\xi_{S=1} \approx 6$.[17] In 2D, we know from the rigorous result[18,19] that the ground state has an LRO, thus it is gapless and $\xi_{S=1} = \infty$. Hence, there should be a QPT at some critical J_y^c from a disordered to an ordered ground state. QMC studies predict $J_y^c \approx 0.04$ (Ref. 20) and $J_y^c = 0.043\,648(8)$.[21] In the two-step study, we applied periodic boundary conditions in the x direction and open boundary conditions in the y direction. In Fig. 2(a) we show the finite-size behavior of the spin gap Δ_s. It shows that in agreement with QMC, J_y^c is located between $J_y = 0.040$ and $J_y = 0.045$. A more accurate DMRG estimate of J_y^c can be obtained by locating the crossing point of consecutive $L_x \times L_y$ systems and extrapolating. But for $S = 1$, an extrapolation was not necessary; for $L_x \times L_y \geqslant 16 \times 17$, the data converged around $J_y^c = 0.043\,68$. We performed the same analysis for coupled $S = 2$ chains. For a single chain $\Delta_{S=2} = 0.0876$ (Ref. 22) and $\xi_{S=2} \approx 49$.[17] The scaled gaps are displayed in Fig. 2(b); we find $J_y^c \approx 0.0007$. It is interesting to note that the values of J_y^c for $S = 1$ and for $S = 2$ are roughly consistent with the Schwinger boson prediction, $J_y^c \times \xi_{1D}^2 \approx J_x$,[23] where ξ_{1D} is the 1D correlation length. We find $J_y^c \times \xi_{1D}^2 = 1.5701$ for $S = 1$, and $J_y^c \times \xi_{1D}^2 = 1.5707$ for $S = 2$. These results suggest that $J_y^c \times \xi_{1D}^2 = \frac{\pi}{2} J_x$. In Fig. 2(c) we show Δ_s for two typical values in a $S = 1$ system, $J_y = 0.02 < J_y^c$ and $J_y = 0.06 > J_y^c$. The extrapolated values are consistent with, respectively, gapped and gapless phases.

In $S = \frac{1}{2}$ two-leg ladders, if the coupling between the rungs is $J_r = J_x = 1$, QMC studies[21] predict that $J_y^c \approx 0.3$. We could not study the QPT because the condition $J_y^c \ll \Delta E$ is not fulfilled. If we reduce J_r enough, the two-step DMRG becomes applicable. This is achieved when $J_r \lesssim 0.5$. For instance, in Fig. 2(d), we display the finite-size behavior of Δ_s for $J_r = 0.4$ and $L_x \times L_y$ ranging from 10×12 to 30×32. For these systems, we find $J_y^c = 0.0993$. An alternative to reducing J_r for $S = \frac{1}{2}$ systems in order to study the QPT in $S = \frac{1}{2}$ systems is increasing the number of legs. When the number of legs increases, Δ_s on the ladder decreases, the system is thus closer to criticality, and therefore a smaller J_y can induce a QPT. For the four-leg ladder with $J_r = 1$, the QMC predicts $J_y^c \approx 0.07$.[24] In Fig. 2(e), we show systems of four-leg ladders ranging from 12×12 to 44×44; it can be seen that $J_y^c \approx 0.08$. In Fig. 2(f), we plot the crossing points of 12×12 and 20×20 to 36×36 and 44×44 systems, respectively. This yields a better estimate of the QCP, $J_y^c = 0.0742$.

Let us now consider the anisotropic Hubbard model defined by hopping parameters $t_x = 1$, $t_y \ll t_x$ and a local interaction U. The noninteracting single-particle energies are $\epsilon_{\mathbf{k}} = -t_x \cos(k_x x) - t_y \cos(k_y y)$, where $\mathbf{k} = (k_x, k_y)$. Since the Fermi surface is nested at the momentum $\mathbf{q_N}$, $\epsilon(\mathbf{k} + \mathbf{q_N}) = -\epsilon(\mathbf{k})$. In the Hartree-Fock approximation, the consequence of nesting is that the metallic state becomes unstable against the formation of a gap $\Delta_c^{\mathrm{HF}} \approx \exp(\frac{-W}{4U})$ and spin-density wave LRO. In 1D, $\Delta_s^{1D} = 0$ for all U and the charge gap $\Delta_c^{1D} \approx \exp(\frac{-W}{4\sqrt{U}})$ for $U/W \ll 1$, and $\Delta_c^{1D} \approx U$ for $U/W \gg 1$. There is no LRO in 1D; the gap opening cannot be explained in the Hartree-Fock approximation. But it is generally believed that the Hartree-Fock approximation is at least qualitatively correct when $t_y \neq 0$.

However, there is a regime of the quasi-1D model where a simple physical argument shows the failure of the Hartree-Fock approximation. If $t_y \ll \Delta_c^{1D}$, interchain motion is prohibited and the electrons are confined into the chains. For any $U > 0$, the system would remain a Mott insulator. There will be an LRO of the Heisenberg type because the spin degrees of freedom are gapless in 1D, and the small t_y would yield an effective exchange, $\tilde{J}_y = t_x^2/\Delta_c^{1D}$. This regime cannot be described by the simple Hartree-Fock theory. This shows that a strong-coupling-like behavior extends even for small U in the confined regime. This somewhat overlooked regime of the Hubbard model was discussed for two-coupled Hubbard chains.[25] It is shown in Ref. 25 that if $t_y \ll \Delta_c^{1D}$, the system is equivalent to the Heisenberg two-leg spin ladder. This is also implicit in the chain dynamical mean-field theory study which predicted that at half filling, a finite t_y was necessary to deconfine the electrons in the transverse direction. Hence, if we increase t_y from the 1D Mott insulator at $t_y = 0$ there are three possibilities: (i) the system remains a Mott insulator; (ii) there is a crossover from a Mott insulator toward a Slater insulator; and (iii) there is a QPT toward a metallic phase.

The two-step DMRG results shown below are consistent with case (iii). In this study, we kept up to $m_1 = 384$ and $m_2 = 96$, respectively, during the first and second steps; the maximum truncation error was less than 1×10^{-7} in the gapped phase, about 1×10^{-5} at the QCP, and 1×10^{-4} in the ordered phase. The bulk of our calculations was

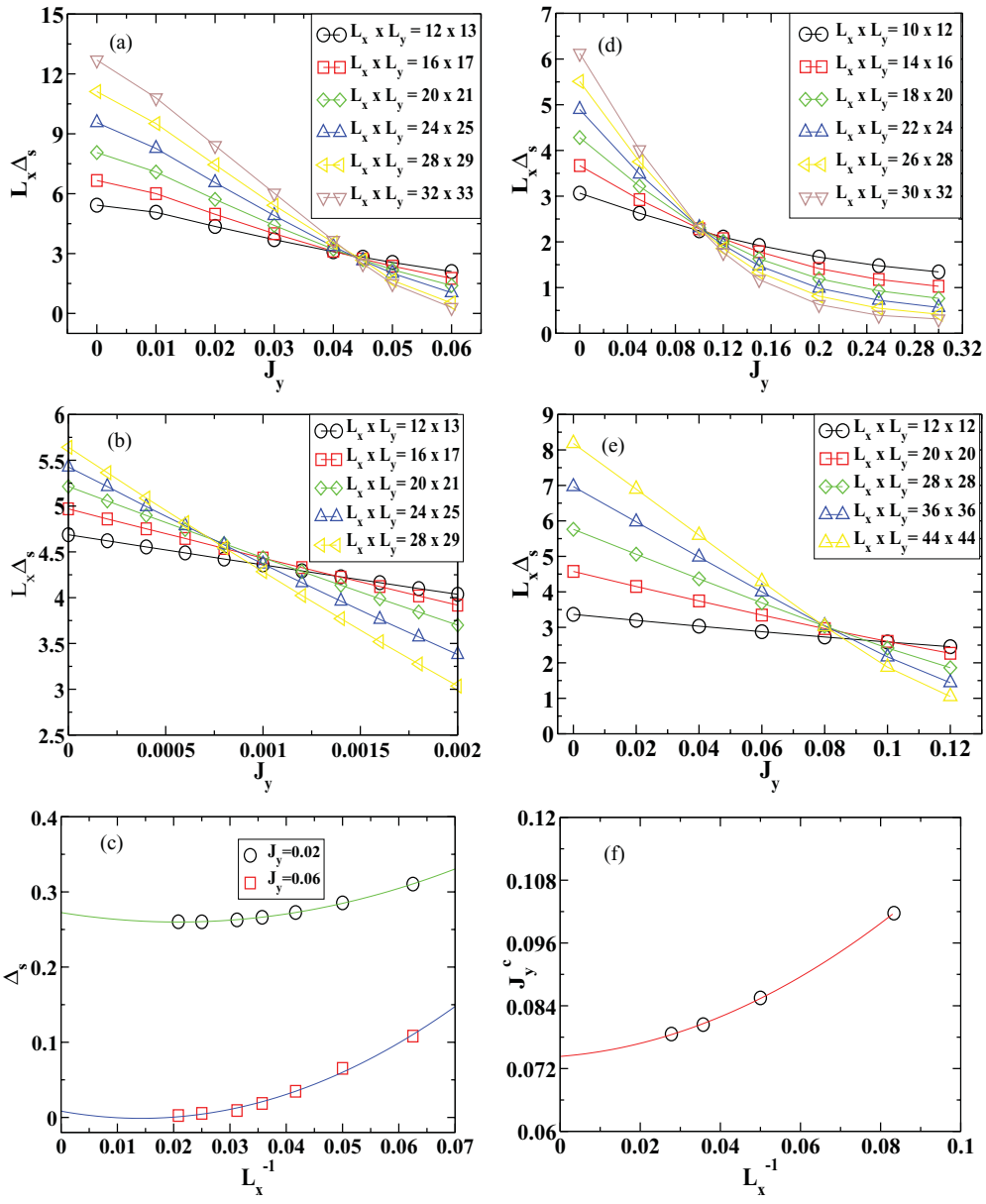

FIG. 2. (Color online) $\Delta_s \times L_x$ as a function of J_y (a) for coupled $S = 1$ chains and (b) for coupled $S = 2$ chains; (c) Δ_s as a function of L_x at two characteristic values below ($J_y = 0.02$) and above ($J_y = 0.06$) the QCP for $S = 1$ chains; (d) $S = \frac{1}{2}$ two-leg ladders at $J_r = 0.4$ (e) and four-leg ladders with $J_r = 1$; and (f) J_y^c as a function of L_x^{-1} in coupled four-leg ladders.

on lattice sizes $L_x \times L_y$ ranging from 12×13 to 32×33, $U = 0,0.5,1,1.5,2,2.5,3$, and at least ten different t_y chosen from $t_y = 0$ to $t_y \approx \Delta_c^{1D}$. In a few cases, 40×41 and 48×49 systems were also studied. In Fig. 3(a) we show the scaled Δ_c as a function of t_y for $U = 1$. The scaled gap displays the typical behavior seen for spin systems. The data for different sizes converge near $t_y = 0.007$. The finite-size behavior of t_y^c (the crossing points of $L_x \Delta_c$ of consecutive systems) is shown in Fig. 3(b). The extrapolation yields $t_y^c = 0.0056$ for $U = 1$. In Fig. 3(c), we display Δ_c as a function of L_x at two typical values of t_y above and below t_y^c. The extrapolated gap is in agreement with the qualitative behavior of $L_x \Delta_c$. Hence Δ_c displays a deconfinement transition from a 1D Mott insulator to a 2D metallic phase. Using the chain-DMFT, Biermann and co-workers[12] find that at $U = 2.6$, the charge correlation exponent K_ρ jumps from 0.02 at $t_y = 0.16$ to 1.01 at $t_y^c = 0.28$. This shows a deconfinement transition with $0.16 \lesssim t_y^c \lesssim 0.28$. We could not however see the t_y induced QPT for $U = 2.6$. The relation $t_y^c \ll \Delta E$ was satisfied only for very small systems. The maximum value for which we could study the t_y-induced QPT is $U = 2$; we find $t_y^c = 0.0689$. We obtain $t_y^c = 0.18$ at $U = 2.6$ by extrapolating from smaller values of U. Since in Ref. 12 they were restricted to paramagnetic solutions, they could not rule out a possible AFM ground state of the Slater type.

Once in the deconfined regime, we can induce a MIT by increasing U. For this purpose, we set $t_y = 0.05$. For this value of t_y we know from the calculations above that for any $U \lesssim 1.5$, the system is in the metallic phase. We thus expect a MIT at some U between $U = 1.5$ and $U = 2$, because as seen

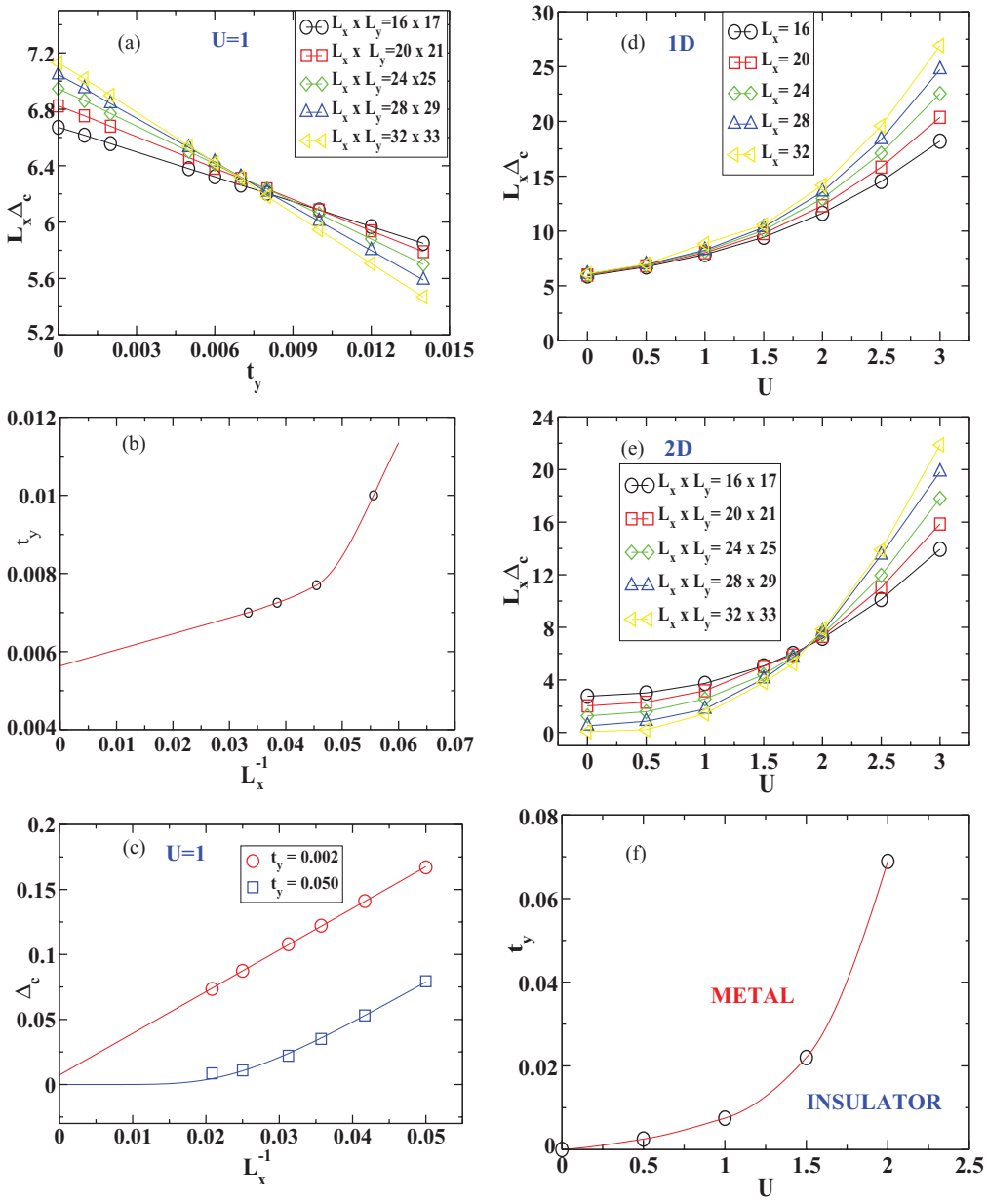

FIG. 3. (Color online) (a) $\Delta_c \times L_x$ as a function of t_y at $U = 1$; (b) the deconfinement transition point t_y^c at $U = 1$ extrapolated from crossing points of two consecutive $L_x \times L_y$; (c) Δ_c as a function of $1/L_x$ at $U = 1$ for two characteristic values of t_y, below ($t_y = 0.002$) and above ($t_y = 0.05$) t_y^c; $\Delta_c \times L_x$ as a function of U in 1D (d) and 2D (e); and (f) phase diagram of the quasi-1D Hubbard model in the (U, t_y) plane.

above, $t_y^c = 0.0689$ at $U = 2$. In Figs. 3(d) and 3(e), we show the scaled Δ_c as a function of U, respectively, in 1D and 2D. In the 2D case [Fig. 3(e)], for $U \lesssim 1.875$, $L_x \Delta_c$ decays when we increase L_x as for $U = 0$ until it reaches $U_c \approx 1.8$ where it starts to increase. This is to be contrasted to the 1D case shown in Fig. 3(d) where there is no regime where $L_x \Delta_c$ decreases when L_x is increased, which implies $U_c = 0$ as we know from the Lieb-Wu solution. In Fig. 3(f), we show the phase diagram of the quasi-1D Hubbard model. The deconfinement transition occurs for small $U \lesssim 1$, at $t_y^c \approx \Delta_c^{1D}/4$.

To conclude, let us comment on the implication of our result on the isotropic case, $t_y = t_x$. For a given U, when $t_y > t_y^c$, the system enters the metallic phase. It should remain in the metallic phase up to $t_y = t_x$, because, as soon as $t_y > t_y^c$, there is no other obvious process that will drive the system to another phase when t_y is further increased. In Ref. 8 the DCA was applied to the isotropic 2D Hubbard model at half filling. It was found, for cluster sizes up to $N_c = 64$, that down to $U = 4$ the paramagnetic solutions remained gapped. Although no gap was found for $U < 4$, it was assumed that the gap would open for larger clusters which were not accessible. However, our result suggests that this assumption may not be true.

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