The metal-insulator transition (MIT), also called the Mott transition\textsuperscript{1}, is certainly one of the most difficult challenges facing condensed matter theorists. Hubbard\textsuperscript{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 quantum fluctuations destroy the Hartree-Fock solution. Therefore, the issue as to whether or not disordered ground states as function of the cluster sizes remains open. 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 non-local fluctuations, the dynamical cluster approximation (DCA)\textsuperscript{3} or the cellular DMFT\textsuperscript{4,5}, have been applied to the 2D Hubbard model. The focus in these studies have 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 function 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 letter, 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)\textsuperscript{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)\textsuperscript{12} at a finite quantum critical point (QCP)\textsuperscript{13}$U/W_c$. This suggests, as seen in the limit of infinite dimensions\textsuperscript{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 coworkers\textsuperscript{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.

Let us briefly describe the two-step DMRG method introduced for coupled chains in Ref.\textsuperscript{11}. This method is generalized here for coupled multi-leg 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: $H = H_{\text{intra}} + H_{\text{inter}} = \sum_i h_i + g H_{\text{inter}}$, where $h_i$ are the Hamiltonians of 1D systems; $g \ll 1$ is the transverse coupling. $H_{\text{inter}}$ is of the same magnitude as $H_{\text{intra}}$. $h_i$ can represent a single chain, a two-leg ladder or even a multi-leg 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 $\phi_n$ and eigenvalues $E_n$ from different charge-spin sectors of the 1D Hamiltonian $h_i$ are obtained by applying the conventional 1D DMRG algorithm\textsuperscript{13}. 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 $\phi_n$'s. Since the resulting effective 2D Hamiltonian is now 1D in the transverse direction, it can be studied using the conventional DMRG. Let for a given size, $E_0$ and $E_{m_2}$ be the lowest and the highest DMRG energies kept for $h_i$. If $g \ll \Delta E = E_{m_2} - E_0$ (in practice we...
set \( \frac{\Delta E}{E} \lesssim 10 \), the two-step DMRG retains high accuracy. But as \( L_x \) increases, \( \Delta E \) decreases, for a fixed \( g \), it would be impossible to retain accuracy for arbitrary 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.

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, \( \Delta(g) \propto (g_c - g)^\nu \), where \( \nu \) is the correlation length exponent (Lorentz invariance is assumed), and \( g_c \) is the value of the gap at the QCP. The product \( L\Delta \), where \( L \) is the linear size of the system is given by a universal function, \( L\Delta = f(C(g_c - g)L^{1/\nu}) \) \(^{14}\), 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 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 systems has a spin gap, the Haldane gap \( \Delta_{S=1} = 0.41049 \) \(^{17}\). The correlation length \( \xi_{S=1} \approx 6 \) \(^{18}\). In 2D, we know from the rigorous result \(^{15,16}\) 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 and ordered ground state. QMC studies predict \( J_y^c \approx 0.04 \) \(^{21}\) and \( J_y^c = 0.043648(8) \) \(^{22}\). In the two-step study, we applied periodic boundary conditions in the \( x \) direction and open boundary conditions in the \( y \) direction. We show in Fig.2(a) the finite size behavior of the spin gap \( \Delta_y \). 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 \( L_x \times L_y \geq 16 \times 17 \), the data converged around \( J_y^c = 0.043613 \). We performed the same analysis for coupled \( S = 2 \) chains. For a single chain \( \Delta_{S=2} = 0.0876 \) \(^{10}\) and \( \xi_{S=2} \approx 49 \) \(^{18}\). 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 bosons prediction, \( J_y^c \times \xi_{1D}^2 \approx J_y \) \(^{20}\), where \( \xi_{1D} \) 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 \( J_y^c \times \xi_{1D}^2 = \frac{3}{2} J_y \). In Fig 2(c) we show \( \Delta_y \) 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 \( J_x = J_x = 1 \), QMC studies \(^{22}\) predict that \( J_y^c \approx \)
increases, \( \Delta \) two-step DMRG becomes applicable. This is achieved closer to criticality, therefore a smaller \( J_y \) is needed. For the four-leg ladder with \( J_r \geq 1 \), the QMC predicts \( J_y^c \approx 0.07 \) [22]. In Fig.2(e), we show systems of four-leg ladders ranging from \( 12 \times 12 \) to \( 44 \times 44 \), it can be seen that \( J_y^c \approx 0.08 \). In Fig.2(f), we plot the crossing points of \( 12 \times 12 \) and \( 40 \times 40 \) to \( 36 \times 36 \) and \( 44 \times 44 \) 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 non-interacting single particle energies are, \( \epsilon_k = -t_x \cos(kx) - t_y \cos(ky) \) where \( k = (k_x, k_y) \). Since the Fermi surface is nested at the momentum \( (q_x, q_y) = -\epsilon(k) \). In the Hartree-Fock approximation, the consequence of nesting is that the metallic state becomes unstable against the formation of a gap \( \Delta^{HF} \approx \exp(-\frac{W}{4U}) \) and spin-density wave LRO. In 1D, \( \Delta^{1D}_c = 0 \) for all \( U \) and the charge gap \( \Delta^{1D}_c \approx \exp(-\frac{W}{4U}) \) 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 \( t_y \ll \Delta^{1D}_c \), inter-chain motion is prohibited, 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, \( J_y = t_y^2/\Delta^{1D}_c \). 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 [24]. It is shown in Ref. [24] that if \( t_y \ll \Delta^{1D}_c \), the systems 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 towards a Slater insulator; (iii) there is a QPT towards a metallic phase.

The two-step DMRG results shown below are consistent with the 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 \( 1 \times 10^{-5} \) in the first step and \( 1 \times 10^{-4} \) in the second step for all the parameters investigated. The bulk of our calculations was on lattice sizes \( L_x \times L_y \) ranging from \( 12 \times 13 \) to \( 32 \times 33 \), \( U = 0 \), \( 0.5 \), \( 1 \), \( 1.5 \), \( 2 \), \( 2.5 \), \( 3 \), and at least 10 different \( t_y \) chosen from \( t_y = 0 \) to \( t_y \approx \Delta^{1D}_c \). In a few cases, \( 40 \times 41 \) and \( 48 \times 49 \) systems were also studied. In Fig.3(a) we show the scaled \( \Delta_c \) as 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 \( t_y^c \approx 0.0056 \) for \( U = 1 \). In Fig.3(c), we display \( \Delta_c \) as function of \( L_x \) at

![Image](https://example.com/image.png)

**FIG. 3:** (a) \( \Delta_c \times L_x \) as function of \( t_y = 1 \); (b) the deconfinement transition point \( t_y^c \) at \( U = 1 \) extrapolated from crossing points of two consecutive \( L_x \times L_y \); (c) \( \Delta_c \) as function of \( 1/L_x \) at \( U = 1 \) for two characteristic values of \( t_y \), below \( (t_y = 0.002) \) and above \( (t_y = 0.05) \); (d) \( \Delta_c \times L_x \) as function of \( U \) in 1D (d) and 2D (e); (f) Phase diagram of the quasi-1D Hubbard model in the \((U, t_y)\) plane.
two typical values of $t_y$ above and below $t'_y$. The extrapolated gap is in agreement with the qualitative behavior of $L_x \Delta_c$. Hence $\Delta_c$ displays a deconfinement transition from a 1D Mott insulator to a 2D metallic phase. Using the chain-DMFT, Biermann and coworkers \cite{12} find that at $U = 2.6$, the charge correlation exponent $K_\rho$ jumps from 0.02 at $t_y = 0.16$ to 1.01 at $t'_y = 0.28$. This shows a deconfinement transition with $0.16 \lesssim t'_y \lesssim 0.28$. We could not however see the $t_y$ induced QPT for $U = 2.6$. The relation $t'_y \ll \Delta E$ 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 $t'_y = 0.0689$. We obtain $t'_y = 0.18$ at $U = 2.6$ by extrapolating from smaller values of $U$. Since in Ref.\cite{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 above $t'_y = 0.0689$ at $U = 2$. In Fig.\(3\)(d),(e), we show the scaled $\Delta_c$ as 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 $t'_y \approx \Delta^{1D}/4$. In a recent experiment, Pashkin and coworkers \cite{25} studied the infrared response of the quasi-1D Fabre salt $(TMTTF)_2PF_6$. Though this compound is nominally three-quarter filled, the presence of small dimerization renders it effectively half-filled. At ambient pressure, $(TMTTF)_2PF_6$ is a Mott insulator. When external pressure is applied, the interchain transfer integral grows exponentially and the Mott gap rapidly decreases until a deconfinement transition is reached. The interchain transfer integral that induces the deconfinement transition is approximately half of the Mott gap. This result is in reasonable agreement with our prediction.

To conclude, let us comment on the implication of our result on the isotropic case, $t_y = t_x$. For a given $U$, when $t_y > t'_y$, the system enters the metallic phase. It should remain in the metallic phase up to $t_y = t_x$, because, as soon as $t_y > t'_y$, there is no other obvious process that will drive the system to another phase when $t_y$ is further increased. In Ref.\cite{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. We reexamined Ref.\cite{8} data, plotting $U_c(N_c)$, where $U_c(N_c)$ is the estimated finite cluster QCP, we find $U_c \approx 3.1$ when $N_c \rightarrow \infty$.

We acknowledge a helpful correspondence with M. Jarrell, R.M. Scalettar, and A.-M.S. Tremblay. We wish to thank A. Schiller for support. This work was supported in part by a Shapiro fellowship of the Israeli Ministry of Immigrant Absorption (S.M.), and by the Israel Science Foundation through grant no. 1524/07.

\begin{thebibliography}{99}

[1] N.F. Mott, Proc. Phys. Soc. (London) A62, 416 (1949).
[2] J. Hubbard, Proc. Roy. Soc.(London) A277, 237 (1964).
[3] E.H. Lieb and F.Y. Wu, Phys. Rev. Lett. 20, 1445 (1968).
[4] W. Metzner and D. Vollhardt, Phys. Rev. Lett. 62, 324 (1989).
[5] A. Georges and G. Kotliar, Phys. Rev. B 45, 6479 (1992).
[6] J.E. Hirsch, Phys. Rev. B 31, 4403 (1984).
[7] C.N Varney, C.-R. Lee, Z.J. Bai, S. Chiesa, M. Jarrell, and R.T. Scalettar, Phys. Rev. B 80, 075116 (2009).
[8] S. Moukouri and M. Jarrell, Phys. Rev. Lett. 87, 167010 (2001).
[9] Y.Z. Zhang and M. Imada, Phys. Rev. B 76, 045108 (2007).
[10] H. Park, K. Haule, and G. Kotliar, Phys. Rev. Lett., 101, 186403 (2008).
[11] S. Moukouri, Phys. Rev. 70, 014403 (2004).
[12] S. Biermann, A. Georges, A. Lichtenstein, and T. Giamarchi, Phys. Rev. Lett. 87, 276405 (2001).
[13] M.N. Barber in 'Phase Transitions and Critical Phenomena', edited by C. Domb and J. L. Lebowitz, Academic Press, London, Vol. 8, p. 145 (1983).
[14] E.J. Neves and J.F. Perez, Phys. Lett. A 114, 331 (1986).
[15] K. Kubo and T. Kishi, Phys. Rev. Lett. 61, 2585 (1988).
[16] O. Golinelli, Th. Jolicoeur, and R. Lacaze, Phys. Rev. B 50, 3037 (1994).
[17] N. Hatano and M. Suzuki, J. Phys. Soc. Jap. 62, 1346 (1993).
[18] X. Wang, S. Qin, Lu Yu, Phys. Rev. B 60, 14529 (1999).
[19] M. Azzouz and B. Doucet, Phys. Rev. B 47, 8660 (1993).
[20] Y. J. Kim and R.J. Birgeneau, Phys. Rev. 62, 6378 (2000).
[21] M. Matsumoto, C. Yasuda, S. Todo, and H. Takayama, Phys. Rev. 65, 014407 (2001).
[22] F.Y. Kim, R.J. Birgeneau, M.A. Kastner, Y.S. Lee, Y. Endoh, G. Shirane, and K. Yamada, Phys. Rev. B 60, 3294 (1999).
[23] K. Lehur, Phys. Rev. B 63, 165110 (2001).
[24] A. Pashkin, M. Dressel, M. Hauke, and C. A. Kuntscher, Phys. Rev. B 81, 125109 (2010).
\end{thebibliography}