On the universality class of the Mott transition in two dimensions

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We use the two-step density-matrix renormalization group method to elucidate the long-standing issue of the universality class of the Mott transition in the Hubbard model in two dimensions. We studied a spatially anisotropic two-dimensional Hubbard model with a non-perfectly nested Fermi surface at half-filling. We find that unlike the pure one-dimensional case where there is no metallic phase, the quasi one-dimensional model displays a genuine metal-insulator transition at a finite value of the interaction. The critical exponent of the correlation length is found to be $\nu \approx 1.0$. This implies that the fermionic Mott transition, belongs to the universality class of the 2D Ising model. The Mott insulator is the 'ordered' phase whose order parameter is given by the density of singly occupied sites minus that of holes and doubly occupied sites.

I. INTRODUCTION

In the studies of the Mott transition[1,2] in the ground state of the Hubbard model[3], there are well controlled results in the pure one-dimensional (1D) case[4] and in the limit of infinite dimensions[5–7] only. In 1D, there is no metallic phase, the Mott gap opens as soon as the interaction $U > 0$. In infinite dimensions, the dynamical mean-field theory which is exact predicts a Mott transition at the critical coupling, $U_c \approx W$, W is the band width. However, the transition has mean-field critical exponents. This anomaly is due to the local nature of the infinite dimensional solution. Hence, the one-dimensional and the infinite dimensional solutions may not be directly applicable to experiments. Studies of the Mott transition in the Hubbard beyond these special limits of one dimension and infinite dimension are thus of crucial importance.

For more than a decade, a great deal of effort has been devoted to applying quantum cluster theories[8–14] to the study of the Mott transition in the Hubbard model in two dimensions (2D). Quantum cluster theories include non-local correlations. They predict a finite critical value for the interaction at the transition. This critical value depends on the cluster size. However, when applied to a finite dimensional model, they are exact only in the limit of infinite cluster size. In quantum cluster theories, the effect of the interaction on physical quantities such as the single-particle Green's function is restricted to the cluster sites. The correlation are fully accounted for distances which are smaller than the cluster length, $r \lesssim L_c$. When $r \gtrsim L_c$, the Green's function has an effective mean-field decay. Restricting the effect of the interaction at distances $r \lesssim L_c$ is probably justified away enough from the critical point where the correlations are expected to be short-ranged. A consequence of this restriction of the correlations to the cluster length is that the exponents at the transition are always mean-field like for a fixed cluster size[10]. A systematic finite cluster size analysis is therefore necessary for a correct description of the transition. However, most of applications of quantum cluster simulations have been done on relatively small clusters.

These are not enough to reliably predict the low-energy physics at the quantum critical point.

Unlike the fermionic model, in the 2D Bose-Hubbard model which displays a transition from a superfluid to a Mott insulator, analytical approaches[15,16] and large scale Monte Carlo simulations[17] have yielded reliable information about its critical behavior. The transition for fixed boson density belongs to the universality class of the classical three-dimensional (3D) XY model. This has also been reported on the 2D Jaynes-Cummings-Hubbard model[18]. Unfortunately, for the fermionic Hubbard model Monte Carlo simulations predict $U_c = 0$. This is because of the nesting induced Slater transition[19,20]. In absence of perfect nesting, the Monte Carlo method is hampered by the sign problem. Large scale simulations are not possible.

Recent interest has been raised by slave rotor analyses[21,22]. These analyses suggest that the transition in the 2D fermionic Hubbard model may belong to the 3D XY universality class as the bosonic Hubbard model. In Ref.[21,22] a slave rotor representation of the fermionic operator $c_{i\sigma} = b_i f_{i\sigma}$, where b_i is a spinless boson and $f_{i\sigma}$ a charge-less spin, was used to map the Hubbard model to a free spinon Hamiltonian self-consistently coupled to a bosonic term (or XY term in a spin representation of bosons). The fermionic Mott transition is in this form a transition between condensed (Fermi liquid) and non-condensed (Mott insulator) phases of bosons. This factorization may be justified in the Mott phase where, because of the Mott gap, spin and charge degrees of freedom may be separated. However, as the critical point is approached, is the gauge field weak enough to justify the decoupling between spin and charge? If not would that modify the critical behavior predicted by the slave-rotor approximation? Only a non-biased calculation of the Hubbard model can yield the answer.

The slave-rotor prediction is in disagreement with an earlier approximate mapping[23] of the Hubbard model to a generalized Blume-Emery-Griffiths model[24] of the $H_e^3 - H_e^4$ mixtures with an additional term whose effect on the nature of the transition is not known. In this mapping, doubly occupied and empty sites corresponds to H_e^4 sites and singly occupied sites to H_e^3 sites. This

mapping suggests instead that the Hubbard model is in the universality class of the Ising model. But the extra term which accompanies the Blume-Emery-Griffiths model could well lead to another universality class.

In a recent paper[25], we reported a two-step density-matrix renormalization group (DMRG)[26] study of the Mott transition in the ground state of the quasi-one-dimensional (1D) Hubbard model at half-filling. We find that in contrast to the pure 1D case for which there is no metallic phase, there is an authentic Mott transition in the quasi-1D model. However, it is possible to argue that in the quasi-1D dimensional Hubbard model studied in Ref.[25], the Fermi surface is perfectly nested, thus our analysis which predicts a gapless phase in the weak-coupling regime, would miss an exponentially small gap $\Delta \propto exp - \frac{2\pi t}{U}$, that would open as a consequence of a Slater transition. However, our numerical data did not support the existence of such a gap. Arguments supporting a gap opening induced by perfect nesting are perturbative: the divergence of the non-interacting susceptibility $\chi_0(\mathbf{q})$ at the nesting wave vector leads to that of the interacting spin susceptibility, $\chi_s(\mathbf{q}) \propto 1/(1 - U\chi_0(\mathbf{q}))$. However, the actual susceptibilities and interaction in the expression of $\chi_s(\mathbf{q})$ are renormalized. Attempts to compute the renormalized susceptibilities and interaction within the self-consistent parquet formalism[27] lead to intractable equations. Hence, the effect of these renormalization effects on the mean-field solution remains an open problem.

In this paper, we present a well controlled study of the Mott transition in the Hubbard model with a non-perfectly nested Fermi surface beyond the special cases of 1D and infinite dimensions. The choice of the non-perfectly nested Fermi surface precludes the theoretical possibility of a gap induced by the Slater anti-ferromagnetism mechanism. The two-step DMRG method is first checked on the transition between a para-magnetic and an anti-ferromagnetic ground states in the quasi-1D Heisenberg model with $S = 1$. In agreement with a quantum Monte carlo study[28], we find that this transition belongs to universality class of the 3D classical Heisenberg model. For the quasi-1D Hubbard model, we find that, in contrast to the pure one-dimensional model, there is a genuine ground-state Mott transition at a finite critical value of the interaction. Data analysis of the critical behavior of this model show that, in agreement with the mapping to the Blume-Emery-Griffiths model[23], the Mott transition in the 2D Hubbard model belongs to the universality class of the 2D Ising model.

II. MODEL

We consider the Hubbard model with the local interaction U and the following non-interacting single-particle energies,

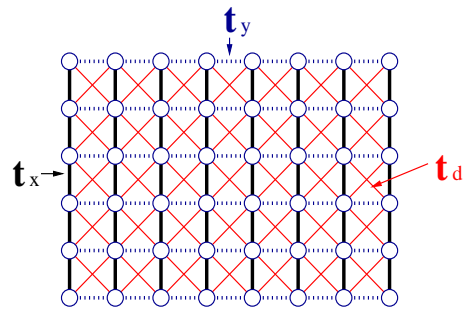$$\epsilon(k_x, k_y) = -2t_x cos k_x - 2t_y cos k_y -$$

FIG. 1: The anisotropic frustrated lattice with longitudinal t_x, transverse t_y, and diagonal t_d hopping parameters.

$$2t_d cos(k_x + k_y) - 2t_d cos(k_x - k_y), \qquad (1)$$

the hopping parameters t_x, t_y, and t_d, respectively in the longitudinal, transverse, and diagonal directions, are illustrated in Fig.1. The presence of t_d ensures that the non-interacting Fermi surface is not perfectly nested. t_y and t_d must be $(t_y, t_d) \ll t_x$ for the two-step DMRG method to be accurate. In this study, we set $t_x = 1$ and $t_y = t_d = 0.05 t_x$. The choice of this model thus precludes the theoretical possibility of the nesting induced exponentially small gap. The band-width is $W = 4.4 t_x$, we set $u = U/W$.

III. TWO-STEP DENSITY-MATRIX RENORMALIZATION GROUP

The two-step DMRG is a generalization of the conventional DMRG method[29] to quasi-1D Hamiltonians. The DMRG is a RG procedure in which the reduced density-matrix is used to retain the most important states of the system. The DMRG itself is a crucial improvement over the block RG method[30] which extended the Wilson RG method[31] used in the solution of the Kondo impurity problem to lattice models. The block method has a major handicap, by dividing the lattice into independent blocks, it neglects at its initial step the inter-block interaction. But if the inter-block interaction is of the same order as the intra-block interaction, this introduces an error from which it is difficult to recover even by keeping a large number of states. In the DMRG the lattice is built by initially coupling the block to the rest of the lattice. Let us consider a system (S) coupled to an environment (E), let N_s and N_e be respectively the number of states respectively of the system and for the environment. Let Φ be for instance the ground-state wave function of the super-system including the system and the environment,

$$\Phi(S, E) = \sum_{i_s=1, N_s; i_e=1, N_e} \alpha_{i_s, i_e} \psi_{i_s} \chi_{i_e}, \qquad (2)$$

where the ψ_{i_s}'s represent the system's basis states and the χ_{i_e}'s the environment basis states; N_s and N_e are re-

spectively the total number of states of the system and of the environment. The essence of the RG procedure is the truncation of the Hilbert's space, starting with a small system for which the total number of states can be kept, at some step when the lattice gets large, only a smaller number $m_s < N_s$ of the system's states can be kept. The error in this truncation is given by the eigenvalues λ_{i_s} of the reduced density-matrix of the system,

$$D_S = \sum_{i_e=1,N_e} \Phi(S,E)\Phi^*(S,E). \tag{3}$$

From the relation,

$$\sum_{i_s=1,N_s} \lambda_{i_s} = 1, \tag{4}$$

the error made by representing the system by m_s states instead of N_s is given by,

$$\rho = 1 - \sum_{i_s=1,m_s} \lambda_{i_s}. \tag{5}$$

For a large number of 1D models, ρ is very small if m_s is only a few hundreds. Application of the DMRG method to Heisenberg chains with $S = 1/2$ or $S = 1^{29}$, $m_s \lesssim 100$, the ground-state energy, correlation functions and lowest excitation gap were obtained with an astonishing accuracy.

It was hoped that, given the level of accuracy of the DMRG for 1D models, the method would also perform reasonably well for 2D models. However, for a 2D lattice, the value of m_s necessary to retain good accuracy appears to increase exponentially with the system size. This is related to the entropy area law which predicts an exponential increase of $m_s \propto 2^{L^{D-1}}$ in 2D. The entropy area law implies that the direct application of the 2D DMRG would only be limited to relatively narrow systems, it however leaves a window of success for quasi-1D systems as we will explain below. The study of quasi-1D models would yield valuable information about the corresponding isotropic models. Most importantly the two-step approach had a direct relevance to the physical properties of quasi-1D materials for which $t_y \ll t_x$ such as the organic and inorganic quasi-1D conductors.

Let us consider for instance the Hubbard chain with a charge gap Δ. If the transverse coupling t_y is infinitely small with respect to Δ, so that the system remains in the same phase as the decoupled chains. It is obvious that the decoupled chain limit is a good starting point to describe the weakly-coupled chain system. As t_y increases, the quality of decoupled chain as a starting point will decrease, if the same number of states is kept, until t_y reaches a quantum critical point t_y^c at which the systems enters in the 2D regime. In principle, when t_y is in the 2D phase, it would be wrong to start from the decoupled chain limit. This is because there are a huge number of low-lying states with nearly equal weight in the reduced density-matrix.

The important point which nevertheless makes calculations possible is that actual calculations are done on finite systems which have a discrete spectrum. Thus even if t_y has a value corresponding to the 2D phase for a system size L, given the discreteness of the energy spectrum for a finite system, if the energy width of the states kept is such that $\Delta E \gg t_y$, starting from decoupled chain might still lead to accurate results. For such a system, the DMRG can be used to study the ground-state phase transition since it will display a different scaling behavior above and below t_y^c. The same type of analysis may be used for gap-less chains as well, $\Delta(L)$ will yield the relevant energy scale above and below the transition.

The separation of the energy scales is basic idea of the two-step DMRG[26]. The two-step DMRG uses the extraordinary accuracy that the DMRG can achieve in 1D in two steps. In the first step, the low-energy Hamiltonian is obtained accurately using the DMRG. Then, in the next step small transverse perturbations are inserted. The 2D effective Hamiltonian is 1D, the DMRG is again applied to solve the problem in the transverse direction. Indeed, this procedure is valid only if the transverse couplings are very small with respect to the longitudinal couplings. The success of the two-step DMRG in yielding reliable results on the eventual new physics induced by the perturbation will depend on the value of the critical transverse coupling necessary to drive the systems in a new phase. If the magnitude of the perturbation t_y necessary to drive the system away from the 1D physics is small in comparison with the width of the states kept, the two-step DMRG is expected to be successful. This is for instance the case of coupled Haldane chains studied in section IV. However, if the magnitude of the perturbation is too large, the two-step DMRG would not be able to describe the 2D physics accurately.

The real challenge in the two-step starts after finishing making the program code work. The essential part of the subsequent activity is finding a region in the parameter space of a given model where interesting physical results can be extracted. For more details about the two-step DMRG, we refer the reader to Ref.[26].

In the first step of the DMRG, we targeted charge sectors with N_e, $N_e \pm 1$, $N_e \pm 2$, where N_e corresponds to the number of electrons at half-filling; for each charge sector, we targeted the spin sectors with the lowest S_z, $S_z \pm 1$; hence we targeted a total of $n_{targ} = 17$ charge-spin sectors during each DMRG iteration. The reduced density-matrix was given by,

$$D_S = \sum_{k=1,n_{targ}} \omega_k \sum_{i_e=1,N_e} \Phi_k(S,E)\Phi_k^*(S,E). \tag{6}$$

where we assigned an equal weight $\omega_k = 1/17$ to each state Φ_k. In all the simulations we kept $ms_1 = 512$ states such that the largest truncation error was $\rho_1 \approx 10^{-6}$ for systems of up to $L_x = 32$ as can be seen in Table I.

	12×13	16×17	20×21	24×25	28×29	32×33
$\Delta E(u=0)$	1.6220	1.2683	1.0410	0.8819	0.7685	0.6772
$\rho_1(u=0)$	8×10^{-9}	3×10^{-7}	7×10^{-7}	1×10^{-6}	3×10^{-6}	4×10^{-6}
$\rho_2(u=0)$	0	0	0	0	0	4×10^{-4}
$\Delta E(u=0.4261)$	1.5630	1.2333	1.0204	0.8733	0.7825	$---$
$\rho_1(u=0.4261)$	1×10^{-7}	3×10^{-7}	7×10^{-7}	1×10^{-6}	2×10^{-6}	$---$
$\rho_2(u=0.4261)$	2×10^{-8}	1×10^{-7}	3×10^{-7}	5×10^{-7}	2×10^{-6}	$---$
$\Delta E(u=0.6818)$	1.6249	1.3121	1.1128	0.9907	0.9134	0.8463
$\rho_1(u=0.6818)$	9×10^{-8}	3×10^{-7}	5×10^{-7}	1×10^{-6}	2×10^{-6}	3×10^{-6}
$\rho_2(u=0.6818)$	2×10^{-8}	8×10^{-8}	1×10^{-7}	2×10^{-7}	2×10^{-7}	7×10^{-7}

TABLE I: Energy width ΔE, truncation errors ρ_1 (first DMRG step), ρ_2 (second DMRG step) for $u = 0$, $u = 0.4261$ (near the quantum critical point), and for $u = 0.6818$ in the Hubbard lattice when $m_1 = 512$ and $m_2 = 96$ states are retained.
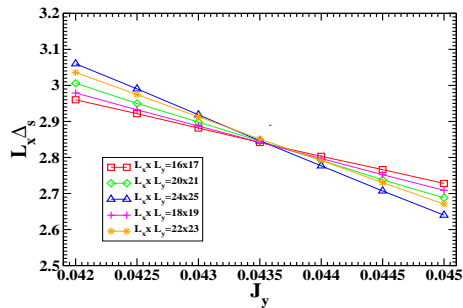

FIG. 2: Scaled spin gap in the quasi-1D Heisenberg model as function of J_y.

In the second step, we targeted $n_{targ} = 3$ charge sectors $N_e, N_e \pm 1$ with the lowest S_z. The reduced density-matrix was formed by attributing an equal weight $\omega_k = 1/3$ for each of $k = 1, n_{targ}$ states. We kept $ms_2 = 96$ states such that the width of the retained states, $\Delta E \gg t_y, t_d$ for $t_d = t_y = 0.05 t_x$. ΔE is displayed in Table I. For these parameters, the truncation error during the second step was such that $\rho_2 \lesssim \rho_1$ for systems of up to $L_x \times L_y = 32 \times 33$ when three superblock states were targeted. We empirically chose ms_2 such that $\Delta E / t_y = 10$. For this ratio, we can accurately reproduce the exact result at $u = 0$.

IV. FINITE-SIZE SCALING

A. General concepts

We apply finite-size scaling[32] to analyze the results on the charge gap Δ. The procedure is simple. We accurately compute Δ in order to locate the quantum critical point. We then collapse the data using the exponents ν of known universality classes in order to find the class corresponding to the Mott transition. We emphasize that in this procedure there is no extrapolation or external parameter besides the data and the exponent of the chosen universality class.

The accurate location of the critical point is done by plotting the product $L_x^{-1}\xi$ as function of the interaction driving the transition. ξ is the correlation length. This is because at the transition, $L_x^{-1}\xi$ is independent of L_x. For the gap the function $L_x^{-1}\xi$ translates to $L_x^{-z}\Delta^{-1}$, where z is the dynamical exponent. Near the the quantum critical point, the product $L_x^z\Delta$ is given by a universal function,

$$L_x^z\Delta = f((g - g_c)L_x^{1/\nu}), \tag{7}$$

where g is a generic coupling driving the transition, g_c is its magnitude at the quantum critical point, and ν is the correlation length critical exponent.

B. Application to coupled Heisenberg chains with $S = 1$

In Fig.2, we illustrate the finite-size analysis that we apply below to weakly coupled Heisenberg chains with $S = 1$. The model which was studied in Ref.[25] is given by the Hamiltonian,

$$H_s = J_x \sum_{i_x,i_y} \mathbf{S}_{i_x,i_y}\mathbf{S}_{i_x+1,i_y} + J_y \sum_{i_x,i_y} \mathbf{S}_{i_x,i_y}\mathbf{S}_{i_x,i_y+1}. \tag{8}$$

In the model (8), there is transition from a magnetically disordered ground state, the Haldane gap phase, to a magnetically ordered ground state which is induced by the transverse coupling J_y. This transition has been studied by the quantum Monte Carlo method[28]. In this transition $z = 1$, and it belongs to the universality class of the 3D classical Heisenberg model, for which $\nu = 0.7048$[33]. In Fig.2 we plot $L_x\Delta_s$ as function of J_y, where Δ_s is the spin gap. We studied systems ranging from $L_x \times L_y = 12 \times 13$ to 24×25. We applied periodic boundary conditions along the x-direction and open boundary conditions along the y-direction. At the quantum critical point $J_y = J_y^c$, $L_x\Delta_s$ is independent of L_x. There are small size effects for smaller systems. We thus included only systems larger than 16×17. All the curves $L_x\Delta_s$ cross at J_y^c. The critical point $J_y^c = 0.04368$ was
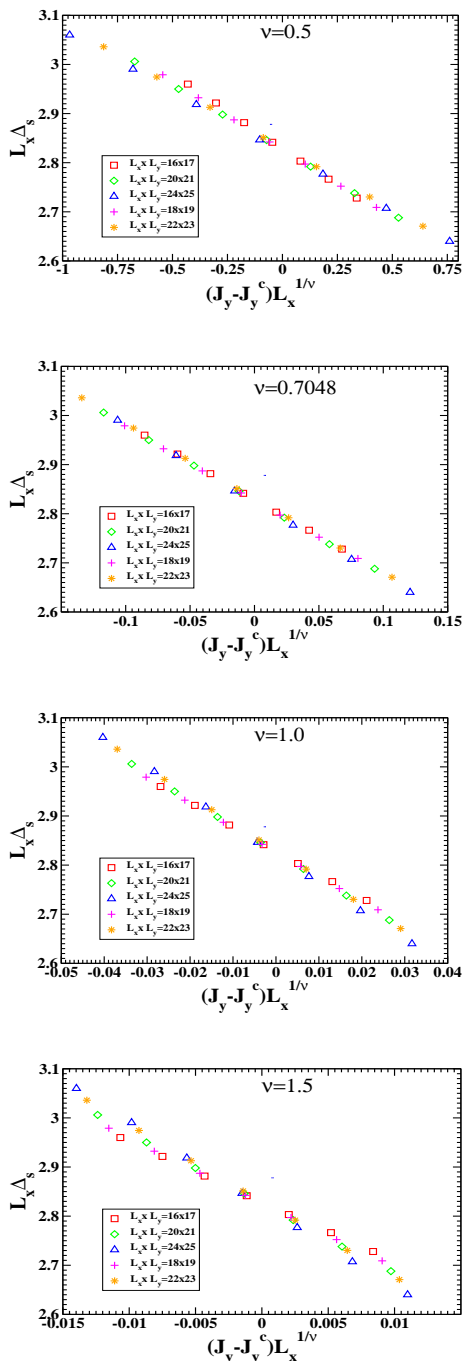
FIG. 3: $\Delta \times L_x$ as function of u ((a) and (b), as function of $(J_y - J_y^c)L_x^{1/\nu}$ for different $L_x \times L_y$ and for different universality classes: mean-field ($\nu = 0.5$), classical 3D Heisenberg ($\nu = 0.7048$), 2D Ising ($\nu = 1.0$), fictitious class ($\nu = 1.5$).

located graphically. It is in perfect agreement with the quantum Monte Carlo value $J_y^c = 0.043648(8)$.

The determination of the universality class is done by plotting $L_x \Delta_s$ as function of $(J_y - J_y^c)L_x^{1/\nu}$. In Fig.3, $L_x \Delta_s$ is displayed for different values of ν corresponding to mean-field, classical 3D Heisenberg, 2D Ising, and a
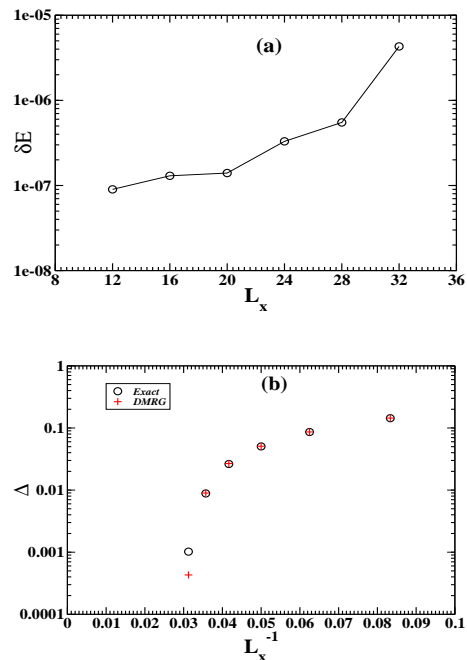

FIG. 4: Error in the ground-state energy for quasi-one-dimensional systems as function of the linear dimension L_x of the lattice. Single-particle two-step DMRG gaps versus exact gaps as function of L_x

fictitious universality class with $\nu = 1.5$. As expected from Monte Carlo simulations, the best data collapse was obtained for $\nu \approx 0.7048$ which is predicted Monte Carlo value[33] for the classical 3D Heisenberg universality class.

V. RESULTS AND DISCUSSION

A. Correlation length exponent at the Mott transition

We can now confidently apply the same method to the Hubbard model. It has roughly the same level of difficulty as the coupled Heisenberg chain problem. First, we compared the two-step DMRG results with the exact energies at $u = 0$. We emphasize that this test is non-trivial for a real-space technique such as the DMRG because in real space, the hopping term is non-diagonal. In Fig.4(a), we show the error δE in the ground-state energies per site for systems ranging from $L_x \times L_y = 12 \times 13$ to 32×33. The two-step DMRG is in very good agreement with the exact result; $\delta E < 10^{-6}$ and increases relatively slowly with L_x for systems $L_x \times L_y < 28 \times 29$ and starts to grow sharply beyond this size. In Fig.4(b), we compare the single-particle gap, $\Delta = \frac{1}{2}[E_0(N+1) + E_0(N-1) - 2E_0(N)]$, obtained with the two-step DMRG to the exact gap. The largest error for the gap was about 5×10^{-4} in the 32×33 systems. Since for this size the exact gap is only $\Delta = 0.00103$, we excluded the 32×33 systems from the
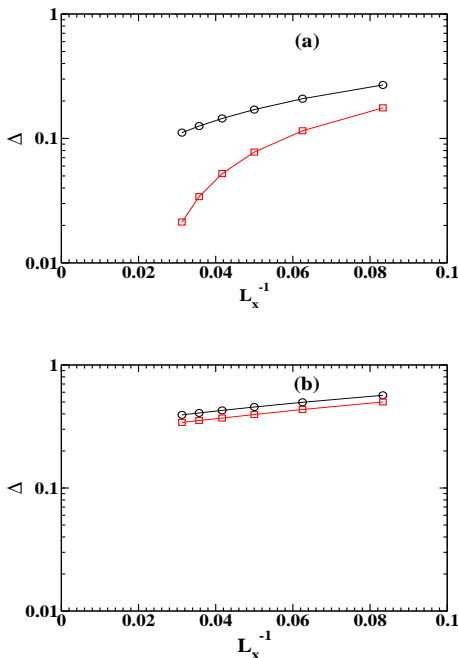
FIG. 5: Quasi-particle gaps as function of L_x for two characteristic values of the interaction: (a) $u = 0.2273$, (b) $u = 0.6818$ for 1D (circles) and quasi-1D (squares) systems.

data used to extract the critical exponent. For the largest systems kept for the analysis 28×29, the two-step DMRG gap is $\Delta = 0.00895$ which is to be compared to the exact gap $\Delta = 0.00883$. The relatively large loss of accuracy in the gap for 32×33 systems follows from the sharp increase in δE.

When $u \neq 0$, the two-step DMRG retains the same level of accuracy as at $u = 0$. This is because, when the same number of states m_2 is kept, the truncation error ρ remains close to that of $u = 0$ as seen in Table I. ΔE slightly increases with u, hence, the condition $\Delta E \gg t_y, t_d$ is also fulfilled. Unlike the pure 1D model, the metallic phase is expected to have a finite width in the quasi-1D model. In Fig. 5 we show the gap as function of L_x for two characteristic values of the interaction at $u = 0.2273$ and $u = 0.6818$ for the 1D and quasi-1D systems. There appears to be two regimes. In Fig.5(a), for $u = 0.2273$ the quasi-1D gap shows a sharp decay in contrast to the 1D gap which decays more slowly. This is consistent with the finite value of the 1D gap and the presumably zero value of the quasi-1D gap in the thermodynamic limit. In Fig.5(b), for $u = 0.6818$ both gaps remain very close and have a finite value in the thermodynamic limit. This behavior suggests that there would be a quantum critical point at $0.2273 \lesssim u_c \lesssim 0.6818$. We would like to emphasize that in Ref.[25], in 1D in agreement with the exact result[4] the DMRG yielded $u_c = 0$.

We analyze our results using the language of second order transitions. This is justified because we did not see any sharp change in our data for the ground-state

energy or the gap. Generally, in a first order transition it would usually be expected that the ground-state energy would be non-differentiable and the gap would show a discontinuity at the transition point. These were not seen in our data. The absence of a discontinuity is seen for instance in the behavior of $L_x\Delta$ in Fig.6. This justifies the assumption that the transition is of second order.

As for the Heisenberg model above, In Ref.[17,18], the value $z = 1$ was predicted for the interaction induced Mott transition. But in the density induced transition the dynamical exponent is $z = 2$. In order to find the value of z, we plotted both $L_x\Delta$ and $L_x^2\Delta$. However, the rough estimate of the critical value found for $L_x^2\Delta$, $u_c \approx 0.1705$ was very inconsistent with the direct extrapolation of the data. For instance, at $u = 0.2273$, Δ extrapolates to 0. This allows us to rule out $z = 2$ as well as higher values of z since they yield even smaller u_c.

We show for $z = 1$, $L_x\Delta$ as function of u in Fig.6. A first sweep of the interaction range $0 \leq u \leq 0.6818$ in Fig.6(a) indicates that $0.4 \leq u_c \leq 0.5$. In Fig.6(b), to precisely locate u_c, we concentrate in the interaction range $0.420 \leq u \leq 0.432$, a graphical estimate yields $u_c = 0.4255$. The range of values of u for the critical analysis $\delta u = 0.02656 u_c$ is comparable to that used in Ref.[17] $|\delta(J/U)| = 0.01526(J/U)_c$ for the Bose Hubbard model, and in Ref.[18] $|\delta(t/g)| = 0.01339(t/g)_c$ for the Jaynes-Cummings-Hubbard model. (J/U) and t/g are the ratio of the hopping parameter over the interaction.

As for the Heisenberg model above, we determine the universality class of the Hubbard model by plotting $L_x\Delta$ as function of $(u - u_c)L^{1/\nu}$. In Fig.7. We tried different values of ν corresponding to the mean-field $\nu = 0.5$, 3D XY, 2D Ising $\nu = 1.0$, and a fictitious $\nu = 1.5$ cases. For the 3D XY model, Monte Carlo values ν are found between $\nu = 0.662(7)$ and $\nu = 0.6723$[34], and with the bosonic Hubbard model[17] and the Jaynes-Cummings-Hubbard model[18] for which $\nu = 0.6715$. The experiments on H_e^4 films are believed to yield the best estimate of ν for the 3D XY models. Experiments have smaller errors than Monte Carlo simulations. For instance ν was found to be $\nu = 0.6708(4)$ in Ref.[35], $\nu = 0.6705(6)$ in Ref.[36], and $\nu = 0.67095(13)$ in Ref.[37]. We used this last value to collapse the data for the test of the 3D XY universality class.

Fig.7, clearly shows that the best fit to the data is obtained for $\nu = 1.0$. This implies that the Mott transition in the Hubbard model belongs to the universality class of the 2D Ising model as predicted by the approximate mapping of Ref.[23].

The 3D XY universality class for the Mott transition in 2D was conjectured in approximate slave-rotor analyses of the fermionic Hubbard model in Ref.[21,22]. This work shows that the neglect of the gauge field during the factorization of the fermionic operators into a spinless boson and a charge-less spin is not justified. It should be noted that the 3D Ising and 3D Heisenberg universality class for which ν is close to that of the 3D XY class, respectively $\nu = 0.6298(5)$[38], $\nu = 0.7048$[33] were also ruled
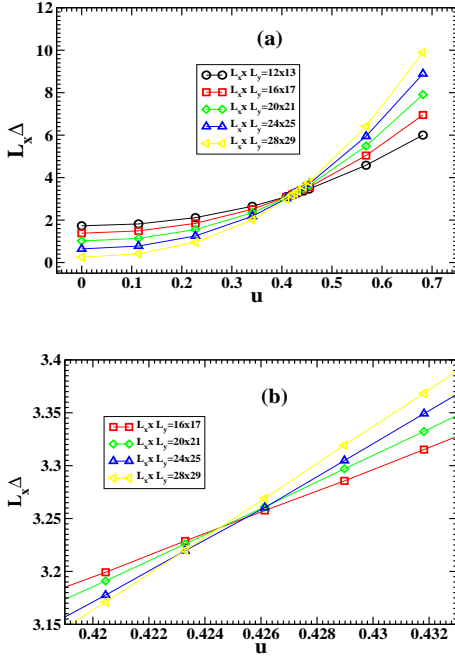
FIG. 6: $\Delta \times L_x$ as function of u for the Hubbard model: (a) extendend range of u, (b) for u in the vicinity of the quantum critical point.

out.

B. Order parameter for the Mott transition

The identification of the universality class of the Mott transition suggests the following analogy with the Ising transition. The weak u limit should correspond to the high temperature phase in the Ising model. At $u = 0$, the four possible local states, $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, and $|\uparrow\downarrow\rangle$ are equally probable respectively with

$$n_0 = \tilde{n}_\uparrow = \tilde{n}_\downarrow = n_d = \frac{1}{4}, \tag{9}$$

in $\tilde{n}_\uparrow$ and $\tilde{n}_\downarrow$ only purely singly occupied sites are counted,

$$\tilde{n}_\uparrow = n_\uparrow - n_d, \tag{10}$$
$$\tilde{n}_\downarrow = n_\downarrow - n_d. \tag{11}$$

In the opposite limit $u = \infty$ which corresponds to the low temperature phase, holes and doubly occupied sites are not allowed,

$$n_0 = n_d = 0, \tag{12}$$
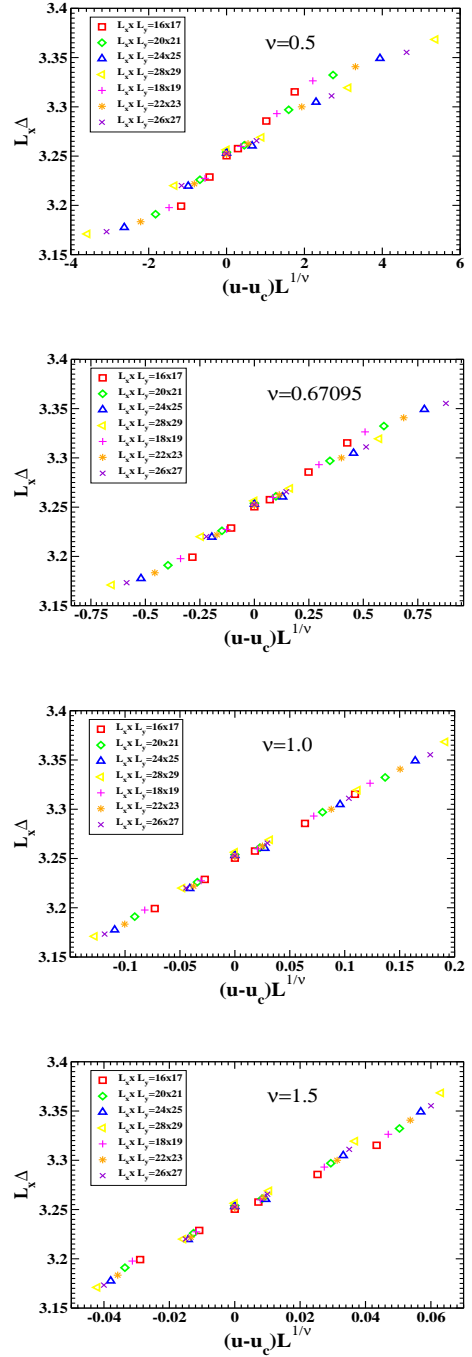$$\tilde{n}_\uparrow = \tilde{n}_\downarrow = \frac{1}{2}, \tag{13}$$

FIG. 7: $\Delta \times L_x$ as function of u ((a) and (b), as function of $(u - u_c)L_x^{1/\nu}$ for different $L_x \times L_y$ for ν corresponding to different universality classes: mean-field ($\nu = 0.5$), 3D classical XY ($\nu = 0.67095$), 2D Ising ($\nu = 1.0$), fictitious ($\nu = 1.5$).

the local possible states have shrinked from 4 to 2 due to the Z_2 Ising symmetry breaking. This is in contrast to the slave-rotor analyses where the Fermi liquid is regarded as the ordered phase. The isomorphism $SU(2)/Z_2 \equiv SO(3)$ implies that in principle after the Mott transition, the effective spin Hamiltonian, obtained

by projecting out the empty and doubly occupied states, should retain the full spin rotational symmetry. The eventual spin long-range order will depend on the couplings present in the effective Hamiltonian.

The natural order parameter M for the Mott transition should thus be given by the average number of singly occupied sites minus the number of doubly occupied and empty sites,

$$M = \langle \tilde{n}_\uparrow + \tilde{n}_\downarrow - n_d - n_0 \rangle. \qquad (14)$$

Thus,

$$M = \langle n - 4n_d \rangle. \qquad (15)$$

For $u = 0$, $M = 0$ and for $u = \infty$, $M = 1$. It should be expected that for $u \leq u_c$, $M = 0$. But this is not true for finite systems. Because of the finite size gap, finite systems are always 'ordered', thus M will always have a finite value for a finite system even when $u \leq u_c$. Since n_d is a local quantity, it changes very slowly with system sizes. This means that very large systems are necessary to extrapolate accurately to its thermodynamic value. In the two-step DMRG approach , it is more judicious to calculate the correlator,

$$M = \frac{1}{L_x}\sqrt{\langle \sum_i M_0 M_i \rangle}, \qquad (16)$$

for the middle chain. M is shown in Fig.8 for a 24×25 system. The curve of M has the usual form of an order parameter curve. However in the vicinity of the quantum critical point, because of the use of open boundary conditions, the data are strongly affected by the 2D remnant of Friedel oscillations. Convergence is very slow even with this definition of M. It can be seen that the value of M is still appreciable at the quantum critical point $u = 0.4255$. Significantly more work will be necessary in order to reliably extract the order parameter exponent β.

VI. CONCLUSION

In this paper, we used the two-step DMRG to analyze the finite size behavior of the quasi-particle gap in the ground-state Mott transition in the quasi-1D Hubbard model. We chose a non-bipartite lattice to avoid the issue related to the possible nesting induced Slater transition. We studied systems ranging from 12×13 to 32×33. We were able to find the universality class of the Mott transition in an un-biased calculation.

In contrast to the pure 1D model, we find that the quasi-1D models displays a genuine Mott transition at a finite critical interaction. Moreover, the quasi-1D solution does not have the pathologies of the infinite dimensional solution. It could thus serve as a basis for more realistic studies of the detailed and well controlled analysis of the Mott transition. The critical behavior of the quasi-1D model Hubbard model is found to belong to the universality class of the 2D Ising model. The fact that the transitions in the quasi-1D Heisenberg and Hubbard models belong to the universality classes of their isotropic counterparts shows that despite the restriction of the two-step DMRG method to highly anisotropic 2D models, it is nevertheless very useful for the understanding of the physics of isotropic 2D systems.

We did not discuss the spin degrees of freedom. They are expected to be gap-less in either side of the Mott transition. In the insulating phase, in the strong coupling limit $U \gg t_x, t_y, t_d$, the anisotropic frustrated Hubbard model is equivalent to the anisotropic $J_1 - J_2$ model with $J_x = t_x^2/U$, $J_y = t_y^2/U$, and $J_d = t_d^2/U$, where J_x, J_y, and J_d are respectively the exchange parameter in the longitudinal, transverse, and diagonal directions. Our choice $t_y = t_d$ implies that the ground state will be magnetically ordered with the momentum $\mathbf{q} = (\pi, 0)$. For intermediate U, in the Mott insulator phase, double occupation is not negligible straighforward mapping to the Heisenberg model is not valid. However, the charge gap opening implies spin-charge separation. Thus even in this case, the effective low-energy Hamiltonian should be Heisenberg like, albeit with non-trivial exchange parameters. Magnetic long-range order should be expected. However, a gap-less spin-liquid ground state with a spinon Fermi surface as suggested in Ref.[21,22] is also possible.
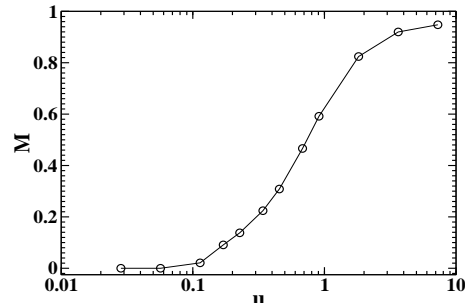
FIG. 8: Order parameter M of the Mott transition as function of u for a 24×25 system.

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