Technische Universität Chemnitz-Zwickau

Sonderforschungsbereich 393

Numerische Simulation auf massiv parallelen Rechnern

R. V. Pai, A. Punnoose, and R. A. Römer

The Mott-Anderson transition in the disordered one-dimensional Hubbard model

Preprint SFB393/97-12

Preprint-Reihe des Chemnitzer SFB 393

SFB393/97-12 **April 1997**

Author's addresses:

Ramesh V. Pai, Department of Physics, Goa University, Goa, 403 206, India,

Alexander Punnoose, Department of Physics, Indian Institute of Science, Bangalore, 560 012, India,

Rudolf A. Römer, Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz

http://www.tu-chemnitz.de/sfb393/

The Mott-Anderson transition in the disordered one-dimensional Hubbard model

Ramesh V. Pai,[1,2] Alexander Punnoose[3] and Rudolf A. Römer[4]

[1]Department of Physics, Goa University, Goa, 403 206, India

[2]Jawaharlal Nehru Center for Advanced Scientific Research, Jakkur, Bangalore, 560 064, India

[3]Department of Physics, Indian Institute of Science, Bangalore, 560 012, India

[4]Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

(Version: April 2, 1997; printed April 24, 1997)

Abstract

We use the density matrix renormalization group to study the quantum transitions that occur in the half-filled one-dimensional fermionic Hubbard model with onsite potential disorder. We find a transition from the gapped Mott phase with algebraic spin correlations to a gapless spin-disordered phase beyond a critical strength of the disorder $\Delta_c \approx U/2$. Both the transitions in the charge and spin sectors are shown to be coincident. We also establish the finite-size corrections to the charge gap and the spin-spin correlation length in the presence of disorder and using a finite-size-scaling analysis we obtain the zero temperature phase diagram of the various quantum phase transitions that occur in the disorder-interaction plane.

71.27+a, 71.30.+h

Typeset using REVTEX

Electronic systems can undergo quantum phase transitions from metallic to insulating behavior as a function of either the interaction strength or the degree of disorder or both [1]. A clean system at certain commensurate fillings may develop a gap in the energy spectrum as the strength of the repulsion is increased and turn into a Mott insulator [2]. On the other hand, a system of noninteracting electrons can undergo a transition from metal to insulator as the degree of randomness is increased and turn into an Anderson localized insulator [3]. The interplay of electron-electron interaction and disorder raises interesting possibilities of a new type of transition, distinct from the clean correlation induced Mott transition or the disorder induced Anderson transition.

The repulsive Hubbard model in one dimension (1D) is probably the simplest model which shows a Mott transition at half-filling for arbitrary values of the interaction strength $U > 0$ [4]. One of the most attractive features of this model is that the Mott transition is unaccompanied by a spin-density-wave gap as *e.g.* happens in the 2D Hubbard model due to the existence of magnetic long-range order (MLRO) [5]. Instead the 1D model shows algebraically decaying spin correlations as the maximal remnant of MLRO in 1D. The properties of the clean 1D Hubbard model are well established: The dependence of the Mott gap on the interaction parameter [4], the asymptotic behavior and the critical exponents of various correlation functions [6] have all been computed using Bethe Ansatz and the finite-size-scaling approach of conformal quantum field theory [7]. All this makes this model particularly attractive to study the effect of disorder on the Mott state.

Recent studies of the half-filled disordered 1D Hubbard model have proceeded numerically using the Quantum Monte Carlo (QMC) method [8] and analytically using bosonization and the renormalization group method [9]. The QMC results give a very accurate description of the finite temperature properties of the system. However, the low temperature properties can only be inferred by extrapolating the finite temperature data and going to larger system sizes. On the other hand, bosonization methods using *perturbative* renormalization group techniques only give an indication of the various plausible fixed points in parameter space. Computing correlation functions at the strong coupling fixed points is then impossible as the coupling constants are driven away from their weak coupling values. Nevertheless, the results of both approaches indicate that at half-filling a *finite* amount of potential disorder is needed to cause a transition from Mott (gapped) to Anderson (gapless) insulating behavior. This is in qualitative agreement with arguments put forward by Ma [10].

In the present Letter, we have studied the ground state properties of the disordered 1D Hubbard model at zero temperature with the help of the density-matrix renormalization group (DMRG) [11]. This method has been previously shown to be highly successful for 1D quantum systems [12,13] and may be seen as a numerical variational-wave-function approach [14]. After introducing the parameters of our DMRG, we show that in the clean case, the previously known results can be reproduced numerically reliably. We then consider finite disorder and show that the charge gap G^c remains open for small disorder up to a critical disorder strength $\Delta_c \approx U/2$. The transition in the spin sector is seen by studying the behavior of the spin-spin-correlation function $\langle S^-(r) S^+(0) \rangle$. For $\Delta < \Delta_c$, the power-law remnant of the MLRO persists, whereas for $\Delta > \Delta_c$, the spin-spin correlation indicates the emergence of a spin-disordered phase.

The Hubbard Hamiltonian with additional potential disorder on a chain of L sites is given as

$$H = -t \sum_{\substack{x=1 \\ \sigma=\uparrow,\downarrow}}^{L} (c^\dagger_{x+1\sigma} c_{x\sigma} + h.c.) + U \sum_{x=1}^{L} n_{x\uparrow} n_{x\downarrow} + \sum_{x=1}^{L} \mu_x n_x, \tag{1}$$

where $-t$ is the hopping amplitude between nearest-neighbor, $c^\dagger_{x\sigma} (c_{x\sigma})$ the fermion creation (annihilation) operator at site x with spin σ, $n_{x\sigma} = c^\dagger_{x\sigma} c_{x\sigma}$ the number operator, $n_x = n_{x\uparrow} + n_{x\downarrow}$ and U is the onsite repulsive energy. The onsite chemical potential μ_x is a random number which we take to be uniformly distributed between $\pm\Delta$ such that $\Delta = 0$ corresponds to the clean case. We work at half-filling, *e.g.* $N = \langle \sum_{x=1}^{L} n_x \rangle = L$ and the energy scale is set by choosing $t = 1$.

We follow the standard open chain DMRG algorithm of White [11]. In each iteration, we diagonalize the Hamiltonian matrix of a super-block denoted by $B^l_{L/2-1} \bullet\bullet\, B^r_{L/2-1}$ of L sites and obtain the energy and the wave function $|\psi_{0L}\rangle$ of the ground state [13]. Here $\bullet$ represents a single site. Using $|\psi_{0L}\rangle$

as the target state [11] we compute the reduced density matrix ρ^l of the left sub-block $B^l_{L/2} \equiv B^l_{L/2-1}\bullet$ of size $L/2$. Diagonalizing ρ^l we obtain its eigenstates and the eigenvalues. These eigenstates with the highest eigenvalues are the most probable states of the left sub-block when the super-block is in the state $|\psi_{0L}\rangle$ and so can be used for truncation. Keeping M eigenstates corresponding to the largest M eigenvalues of ρ^l as the new basis of the left sub-block, we transform the Hamiltonian and all further operators into this new basis. Since every single $\bullet$ has 4 states, we thus truncate the original $4M$ states of $B^l_{L/2}$ to only M states. Usually we have used $M = 128$. Because the disorder destroys translational symmetry, the left and right sub-blocks are non-identical. Hence a similar procedure needs to be followed for the right sub-block $B^r_{L/2}$. The above steps are then repeated for the new super-block $B^l_{L/2}\bullet\bullet B^r_{L/2}$ with $L+2$ sites and thus the system increases by two sites at each iteration.

Let $E_0(L)$ denote the ground state energy of the Hubbard chain of length L with $N_\uparrow = N_\downarrow = L/2$. In order to compute the charge gap G^c_L for a system of finite length L, we repeat the DMRG steps with $N_\uparrow = L/2+1$ and $N_\downarrow = L/2$ and also with $N_\uparrow = L/2-1$ and $N_\downarrow = L/2$. We denote these two ground state energies by $E_1(L)$ and $E_{-1}(L)$, respectively. The charge gap is then defined as the discontinuity of the chemical potential at half-filling [4], *i.e.*, $G^c_L = E_1(L) + E_{-1}(L) - 2E_0(L)$. In the presence of disorder G^c_L is computed for at least 10 different disorder realizations and then averaged over all such realizations. We also compute the spin-spin-correlation function $\Gamma^s_L(r) = \langle\psi_{0L}|S^-(r)S^+(0)|\psi_{0L}\rangle$ and the second moment of the staggered antiferromagnetic (AFM) correlation function $(\xi^s_L)^2 = \sum_r r^2(-1)^r\Gamma^s_L(r)$. Here, $S^+(r) = c^\dagger_{r\uparrow}c_{r\downarrow}$. In the presence of disorder, the correlation functions are first averaged over the disorder realizations and then the correlation length ξ^s_L of the averaged staggered correlation function is found.

The clean case $\Delta = 0$: It has been shown in Ref. [4] that the half-filled repulsive 1D Hubbard model exhibits a charge gap for all non-zero values of the interaction strength. We find that the functional dependence of the thermodynamic value of the charge gap G^c_∞ on the interaction strength U as obtained by DMRG (Fig. 1) is in excellent agreement with the exact solution computed in Ref. [4],

$$G^c = U - 4 + 8\int_0^\infty dw \frac{J_1(w)}{w(1+\exp{(wU/2)})} \tag{2}$$

with $J_1(w)$ a Bessel function. We note that the DMRG algorithm using open boundary conditions gives consistent results for the extrapolated charge gap G^c_∞ with that of Eq. 2 which has been derived using periodic boundary conditions. Nevertheless, we now employ a finite-size-scaling (FSS) analysis of the charge gap G^c_L in order to remove any finite-size effects that could arise in the extrapolation. In Fig. 1 (inset) we show that the leading order finite-size corrections to G^c_∞ fall off as $1/L$, *i.e.* $G^c_L(U) = G^c_\infty(U) + g(U)/L$. Having determined the explicit scale dependence of G^c_L, a plot of LG^c_L versus U as in Fig. 2 shows curves for different L coalescing as the charge gap vanishes. This finite-size behavior allows a numerically accurate determination of the critical value of the interaction strength and we find in accordance with the result of Ref. [4] that the Mott transition occurs at $U = 0$.

The disordered case $\Delta \neq 0$: Quantum Monte Carlo [8] and bosonization [9] studies have predicted the existence of a critical disorder $\Delta_c > 0$ beyond which the Mott gap vanishes. In the limit of large U, this can be motivated [15] by potential energy considerations: any rearrangement of the one particle per site configuration in the half-filled Hubbard model would necessarily cost an energy U due to double occupancy and would gain in the local site potential energy a maximum of 2Δ. Hence, in order for it to be feasible for the electrons to take advantage of the random site energies we should have $\Delta_c \geq U/2$ in the case of bounded disorder. In Fig. 3 we show G^c_∞ as a function of the disorder strength Δ for $U = 2$. We see that the system undergoes a transition from a gapped Mott insulator phase to a gapless phase for $\Delta_c \approx 1 = U/2$. Fig. 3 (inset) shows the finite-size corrections to G^c_∞ in the presence of two representative weak ($\Delta = 0.1$) and strong ($\Delta = 1.0$) disorder strengths for $U = 2$. We note that the corrections continue to fall off as $1/L$ even in the presence of disorder. The FSS plot of LG^c_L versus Δ (Fig. 4) shows that curves for different L coalesce at $\Delta_c = 1.0 \pm 0.1$ again indicating the transition from a gapped to a gapless phase as the strength of the disorder is increased. We have also done the same analysis for $U = 3$ and 5 where a well developed Mott gap exists and where the DMRG is more stable [11]. Our results indicate that the transition into the gapless phase takes place at $\Delta_c \approx U/2$.

Spin-spin-correlation function: For $\Delta = 0$, the half-filled 1D Hubbard model shows algebraically decaying antiferromagnetic (AFM) correlations as computed by the methods of conformal field theory and bosonization [6],

$$\Gamma^s(r) \approx A_1 \frac{\cos(\pi r + \phi_1)}{r} + \mathcal{O}(1/r^2), \quad (3)$$

When the spin-spin-correlation function decays as a power-law, as in Eq. 3, the AFM correlation length ξ^s_∞ diverges in the thermodynamic limit. However, in the absence of long-ranged correlations, ξ^s_∞ remains finite. Fig. 5 (inset) shows that for $\Delta = 0.1$ the finite-size correction to $1/\xi^s_\infty$ continues to fall off as $1/L$ such that $1/\xi^s_L(\Delta) = 1/\xi^s_\infty(\Delta) + \zeta(\Delta)/L$ and we can also apply the previous FSS analysis to the correlation length. In Fig. 5 we plot L/ξ^s_L as a function of Δ. The data for different L coalesce until the disorder $\Delta_s \approx 0.9 \pm 0.1$. Thus for $U = 2$ the staggered $\Gamma^s(r)$ continues to fall off with a power-law up to this critical disorder Δ_s. For larger Δ beyond Δ_s, the values of L/ξ^s_L do not coalesce any more. This indicates the transition from power-law correlations into a short-ranged spin-disordered phase with a finite correlation length. Again, the same analysis of the spin-spin-correlation function for $U = 3$ and 5 confirms that $\Delta_s \approx U/2$.

Thus the two transitions seen above viz. (I) gapped Mott insulator phase to a gapless phase at Δ_c and (II) long-ranged AFM phase to a short-ranged spin-disordered phase at Δ_s, are coincident, and $\Delta_c = \Delta_s$ within the numerical accuracy. Beyond the critical disorder $\Delta_c \approx U/2$ the gapped Mott insulator with power-law AFM correlations goes over to a gapless short-ranged spin-disordered phase. This is the main result of our work and allows us to show in Fig. 6 the phase diagram of the zero temperature quantum transitions that occur in the 1D disordered half-filled Hubbard model.

In summary, the DMRG allows us to analyze the various quantum transitions that occur in the half-filled 1D Hubbard model in the presence of onsite disorder. For $\Delta = 0$ we find that the finite-size corrections to the thermodynamic value of the charge gap G^c_∞ scale as $1/L$ (Fig. 1 (inset)). The functional dependence of $G^c_\infty(U)$ on the interaction strength (Fig. 1) is in excellent agreement with the exact solution computed in Ref. [4] in support of our DMRG approach. We have further shown that for $\Delta \neq 0$, the finite size corrections to $G^c_\infty(\Delta)$ continue to fall off as $1/L$. For small $\Delta < U/2$, the Mott gap is shown to survive. Curves of LG^c_L versus Δ for different L (Fig. 4) come together at Δ_c (≈ 1.0) and coalesce after that indicating a transition from the gapped Mott insulator phase to a gapless phase. A finite-size analysis of the staggered AFM correlation length ξ^s_L shows that the values of L/ξ^s_L for various disorders Δ (Fig. 5) also coalesce at $\Delta_s \approx 1.0 \pm 0.1$. These transitions in the charge and the spin sector are shown to be coincident $\Delta_c = \Delta_s$. Thus in the gapped Mott phase $\Gamma^s(r)$ decays algebraically and is short ranged in the disordered gapless phase. We obtain the (U, Δ) phase diagram (Fig. 6) showing the phase boundary which separates the gapped Mott insulator phase with algebraic spin correlations and the spin-disordered gapless phase.

ACKNOWLEDGMENTS

We sincerely thank S. Ramashesha for useful discussions on the DMRG technique and the HRZ (TUCZ) and SERC (IISc) for the computing facilities. This work has been supported by the Deutsche Forschungsgemeinschaft (Sfb 393).

REFERENCES

[1] For a review, see, P. A. Lee and T. V. Ramakrishnan, Rev. Mod. Phys. **57**, 287 (1985); D. Belitz and T. R. Kirkpatrick, Rev. Mod. Phys. **66**, 261 (1994).

[2] N. F. Mott, *Metal-Insulator Transitions*, Taylor & Francis, (London 1990).

[3] P. W. Anderson, Phys. Rev. **109**, 1492 (1958).

[4] E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).

[5] S. R. White, D. J. Scalapino, R. L. Sugar, E. Y. Loh, J. E. Gubernatis, and R. T. Scalettar, Phys. Rev. B **40**, 506 (1989).

[6] F. Woynarovich, J. Phys. A **22**, 4243 (1989); H. Frahm and V. E. Korepin, Phys. Rev. B **42**, 10553 (1990); H. J. Schulz, Phys. Rev. Lett. **64**, 2831 (1990);

[7] A. A. Belavin, A. M. Polyakov, and A. B. Zamolodchikov, Nucl. Phys. **B241**, 333 (1984); J. L. Cardy, Phys. Rev. Lett. **52**, 1575 (1984).

[8] A. W. Sandvik, D. J. Scalapino and P. Henelius, Phys. Rev. B **50**, 10474 (1994).

[9] S. Fujimoto and N. Kawakami, preprint (1996, cond-mat/9609011).

[10] M. Ma, Phys. Rev. B **26**, 5097 (1982).

[11] S. R. White, Phys. Rev. Lett. **69**, 2863 (1993).

[12] For a brief review, see, G. A. Gehring, R. J. Bursill, and T. Xiang, preprint (1996, cond-mat/9608127).

[13] R. V. Pai, R. Pandit, H. R. Krishnamurthy, and S. Ramasheshа, Phys. Rev. Lett. **76**, 2937 (1996).

[14] S. Östlund and S. Rommer, Phys. Rev. Lett. **75**, 3537 (1995).

[15] R. Shankar, Int. J. Mod. Phys. B **4**, 2371 (1990).

FIGURES

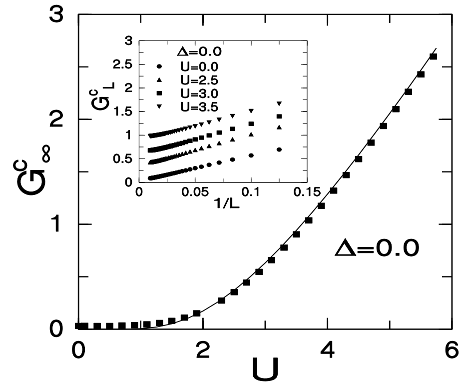

FIG. 1. Filled squares (■) show the charge gap G^c_∞ as a function of the interaction strength U. The exact result [4] is shown by the solid line. Inset: G^c_L vs $1/L$ for $U = 0.0, 2.5, 3.0$ and 3.5. The value of the intercept gives G^c_∞.

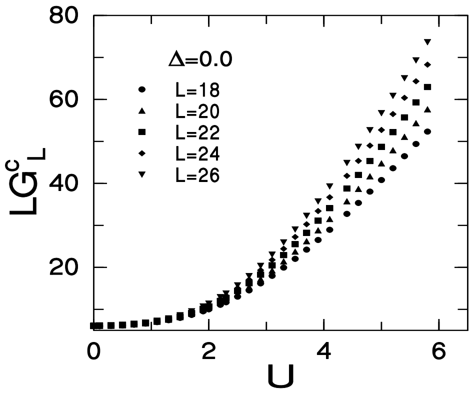

FIG. 2. LG^c_L as a function of the interaction strength U showing the coalescence of curves for different L at $U = 0$. This indicates that the critical value of the interaction strength at which the Mott transition occurs is $U = 0$.

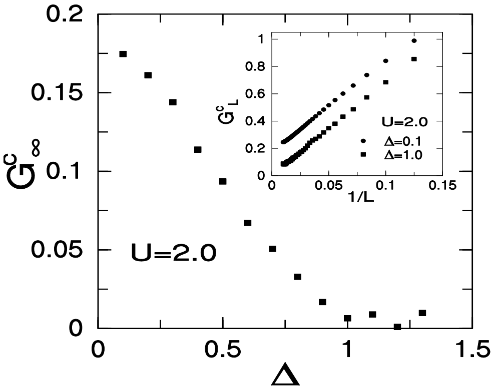

FIG. 3. Filled squares (■) show the charge gap G^c_∞ as a function of the disorder Δ for $U = 2$. Inset: G^c_L vs $1/L$ for $\Delta = 0.1$ and 1.0. The value of the intercept gives G^c_∞.

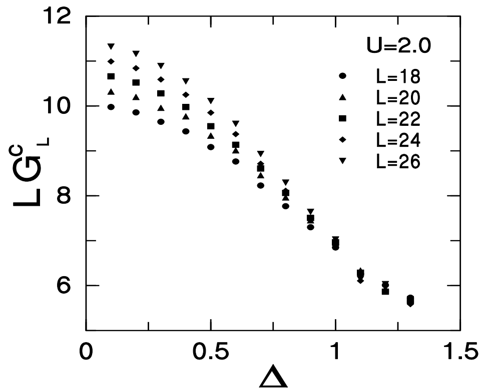

FIG. 4. LG^c_L as a function of the disorder Δ for $U = 2$ showing the coalescence of the curves for different L at $\Delta = 1.0$. This indicates the transition from a gapped Mott insulator phase to a gapless phase.

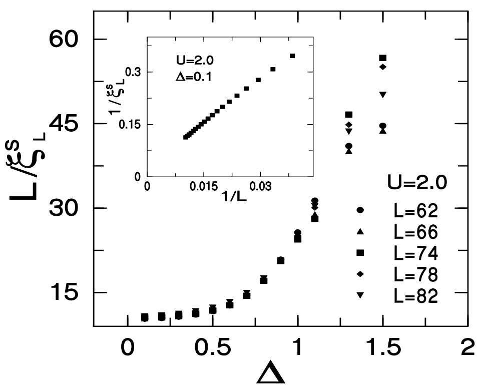

FIG. 5. L/ξ_L^s as a function of the disorder Δ for $U = 2$ showing the coalescence of the curves for different L at $\Delta \approx 0.9 - 1.0$. This indicates the transition from a gapped Mott insulator phase to a spin-disordered gapless phase. Inset: $1/\xi_L^s$ vs $1/L$ for $\Delta = 0.1$.

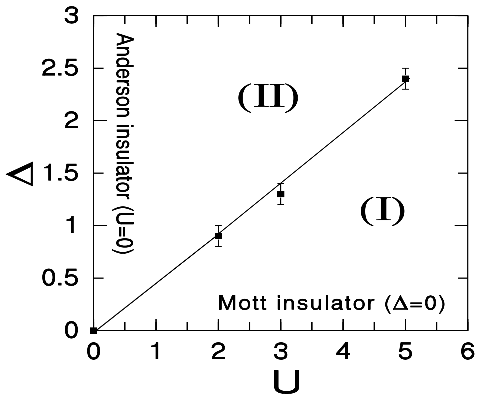

FIG. 6. The phase diagram of the disordered 1D Hubbard Hamiltonian (1) at half-filling showing the Mott insulator with algebraic spin correlations (I) and the gapless spin disordered phase (II). The phase boundary has been drawn through the computed points (filled squares (■) with error bars) and is close to $\Delta = U/2$.