Insulator-Metal Transition in the One- and Two-Dimensional Hubbard Models

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We use quantum Monte Carlo methods to determine $T = 0$ Green functions, $G(\vec{r}, \omega)$, on lattices up to 16×16 for the 2D Hubbard model at $U/t = 4$. For chemical potentials μ within the Hubbard gap $|\mu| < \mu_c$ and at *long* distances $\vec{r}$, $G(\vec{r}, \omega = \mu) \sim e^{-|\vec{r}|/\xi_l}$ with critical behavior $\xi_l \sim |\mu - \mu_c|^{-\nu}$, $\nu = 0.26 \pm 0.05$. This result stands in agreement with the assumption of hyperscaling with correlation exponent $\nu = 1/4$ and dynamical exponent $z = 4$. In contrast, the generic band insulator as well as the metal-insulator transition in the 1D Hubbard model are characterized by $\nu = 1/2$ and $z = 2$. [S0031-9007(96)00052-X]

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At zero temperature a continuous metal-insulator transition (MIT) driven by a change in chemical potential may be characterized by the compressibility, χ_c, or the Drude weight, D. In the Mott insulating phase both D and χ_c vanish, while they remain finite in the metallic phase [1,2]. In order to describe the MIT from the insulator side, we propose to consider the zero-temperature Green function $G(\vec{r}, \omega)$ [3]. At *long* distances, $|\vec{r}|$, and for values of the chemical potential, μ, within the charge gap, namely, $|\mu| < \mu_c$, $G(\vec{r}, \omega = \mu) \sim e^{-|\vec{r}|/\xi_l}$. The MIT may be characterized by the divergence of ξ_l as the critical chemical potential, μ_c, is approached from the insulating phase. ξ_l may be interpreted as the localization length involved in transferring a particle over a distance $\vec{r}$ from the electronic system to the heat bath lying at energy μ within the charge gap. In this Letter, based on a recently developed numerically stable quantum Monte Carlo (QMC) algorithm to calculate zero-temperature imaginary time Green functions [4], we calculate ξ_l for the two-dimensional (2D) repulsive Hubbard model at $U/t = 4$. A great advantage of studying the MIT by approaching it from the insulating phase is that the QMC method does not suffer from the negative sign problem, and hence proves to be a powerful tool, especially for ground state properties. Using this approach for the first time to estimate critical exponents of the MIT, we obtain the following accuracy: $\mu_c = 0.67 \pm 0.015$ in units of the hopping matrix element and $\xi_l \sim |\mu - \mu_c|^{-\nu}$ with $\nu = 0.26 \pm 0.05$. This result corresponds to the first direct determination of the exponent ν and provides unambiguous numerical evidence that the Mott transition in the 2D Hubbard model belongs to a novel universality class. Under the assumption of hyperscaling, this universality class is characterized by a correlation length exponent $\nu = 1/4$ and dynamical exponent $z = 4$ [2]. In contrast, the generic band insulator in all dimensions, as well as the Mott transition in the 1D Hubbard model, satisfy the hyperscaling assumption with exponents $\nu = 1/2$ and $z = 2$ [2,5–7].

The Hubbard model we consider reads

$$H - \mu N = -t \sum_{\langle \vec{i}, \vec{j} \rangle, \sigma} c^{\dagger}_{\vec{i},\sigma} c_{\vec{j},\sigma} + U \sum_{\vec{i}} \left(n_{\vec{i},\uparrow} - \frac{1}{2} \right) \left(n_{\vec{i},\downarrow} - \frac{1}{2} \right) - \mu \sum_{\vec{i},\sigma} c^{\dagger}_{\vec{i},\sigma} c_{\vec{i},\sigma} \,. \tag{1}$$

Here, $\langle \vec{i}, \vec{j} \rangle$ denotes nearest neighbors. $c^{\dagger}_{\vec{i},\sigma}$ ($c_{\vec{i},\sigma}$) creates (annihilates) an electron with z component of spin σ on site $\vec{i}$ and $n_{\vec{i},\sigma} = c^{\dagger}_{\vec{i},\sigma} c_{\vec{i}\sigma}$. In this notation, half-band filling corresponds to $\mu = 0$. We start by considering the noninteracting case, $U/t = 0$. In Fourier space, the single-particle energies are given by $\epsilon_{\vec{k}} = -2t[\cos(\vec{k}\vec{a}_x) + \cos(\vec{k}\vec{a}_y)]$, $\vec{a}_x$, $\vec{a}_y$ being the lattice constants. The length scale is set by $|\vec{a}_x| = |\vec{a}_y| = 1$. At zero temperature, an insulator-metal transition will occur when $\mu \to \mu_c = 4t$. For those chemical potentials, the zero-temperature Green function [3] at $\omega = \mu$ is given by

$$G(\vec{r}, \omega = \mu) = \frac{2}{N} \sum_{\vec{k}} \frac{e^{i\vec{k}\cdot\vec{r}}}{\epsilon_{\vec{k}} - \mu} \,, \tag{2}$$

where N denotes the number of sites of the square lattice and the factor 2 corresponds to the summation over the spin degrees of freedom. Numerically, one obtains $G(\vec{r}, \omega = \mu) \sim e^{-|\vec{r}|/\xi_l}$ with critical behavior $\xi_l \sim |\mu - \mu_c|^{-1/2}$ [8]. As will be discussed below, this example of a band insulator-metal transition satisfies the hyperscaling assumption with exponents $\nu = 1/2$ and $z = 2$. At finite values of U/t and half-band filling the antiferromagnetic Hartree-Fock approximation equally yields $\xi_l \sim |\mu - \mu_c|^{-1/2}$. However, this approximation does not satisfy the hyperscaling assumption.

The physical interpretation of ξ_l is facilitated by considering the single impurity Hamiltonian (Fano-Anderson model) [9,10]:

$$H = \sum_{\vec{k}} \epsilon_k c^{\dagger}_{\vec{k}} c_{\vec{k}} + \epsilon_b b^{\dagger} b + \frac{t_b}{\sqrt{N}} \sum_{\vec{k}} \left(c^{\dagger}_{\vec{k}} b + b^{\dagger} c_{\vec{k}} \right). \tag{3}$$

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Here, $b^\dagger$ creates an electron in the impurity state at the origin and energy ϵ_b. The hybridization between the localized state and the band electrons alters the energy of the impurity level to the value $E_b = \epsilon_b + (t_b^2/N)\sum_{\vec{k}}[1/(E_b - \epsilon_{\vec{k}})]$. We will assume $E_b > \epsilon_{\vec{k}}$ for all $\vec{k}$. When all single particle states of the valence band are filled and the impurity single particle state empty, the probability amplitude of transferring a band electron at site $\vec{r}$ to the impurity state is

$$\frac{\langle\Psi_0|b^\dagger c_{\vec{r}}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} = -\alpha(E_b)\frac{t_b}{N}\sum_{\vec{k}}\frac{e^{i\vec{k}\cdot\vec{r}}}{\epsilon_{\vec{k}} - E_b}, \quad (4)$$

where the normalization factor is given by $\alpha^{-1}(E_b) = 1 + (t_b^2/N)\sum_{\vec{k}} 1/(E_b - \epsilon_{\vec{k}})^2$. Comparison between Eqs. (4) and (2) shows that the spatial dependence of the two quantities is identical. ξ_l may thus be interpreted as the localization length involved in transferring a particle over a distance $\vec{r}$ from the valence band to the heat bath [see Eq. (2)], or to the impurity state [see Eq. (4)]. This definition of ξ_l bears some similarity to that applied in finite size scaling studies of Anderson localized states [11,12]. When the imaginary part of the Green function vanishes in the insulating phase, ξ_l may be used to study the MIT.

To obtain an estimate of the critical exponent ν for the Hubbard model, we require an accurate determination of the critical chemical potential, μ_c, as well as of the localization length, ξ_l. Both quantities may be obtained from the knowledge of

$$G_\sigma(\vec{r},\tau) = \Theta(\tau)\frac{\langle\Psi_0|c_{\vec{r},\sigma}(\tau)c^\dagger_{\vec{0},\sigma}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} - \Theta(-\tau)\frac{\langle\Psi_0|c^\dagger_{-\vec{r},\sigma}(-\tau)c_{\vec{0},\sigma}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}, \quad (5)$$

where $c_{\vec{r},\sigma}(\tau) = e^{\tau H}c_{\vec{r},\sigma}e^{-\tau H}$. Here, $|\Psi_0\rangle$ denotes the ground state of the half-filled ($\mu = 0$) Hubbard Hamiltonian (1). The above quantity may be efficiently calculated with QMC methods. Since we are at half-band filling, the sign problem does not occur, and we are able to consider lattice sizes up to linear dimension $L = 16$, namely, $N = 16 \times 16$ without any serious difficulties. The calculation of imaginary time Green function in the zero-temperature auxiliary field QMC algorithm [13,14] was first reported by Deisz *et al.* [15]. However, their approach does not incorporate a numerical stabilization scheme, and they are thus restricted to small values of τ (i.e., $\tau t \sim 2.5$). Based on ideas used for the stabilization of finite temperature QMC algorithms [16], the authors have developed a numerically stable QMC algorithm for the calculation of $G_\sigma(\vec{r},\tau)$. The details of the algorithm may be found in Ref. [4]. All our calculations were performed with periodic boundary conditions.

From the knowledge of $G_\sigma(\vec{r},\tau)$ on an N-site lattice, we may obtain an estimate of the charge gap. We denote by $|\Psi_n^N\rangle$ the eigenvector of the Hamiltonian H with eigenvalue E_n^N in the N-particle Hilbert space. With this notation,

$$G(\vec{r}=0,\tau) \equiv \sum_\sigma G_\sigma(\vec{r}=0,\tau) = \frac{1}{N}\sum_{n,\vec{i},\sigma}|\langle\Psi_0^N|c^\dagger_{\vec{i},\sigma}|\Psi_n^{N+1}\rangle|^2 \times \exp[-\tau(E_n^{N+1} - E_0^N)] \quad (6)$$

for $\tau > 0$. Figure 1(a) plots $G(\vec{r} = 0,\tau)$ for a 16×16 lattice at $U/t = 4$. We may obtain a reliable estimate of the charge gap for this lattice size by fitting $G(\vec{r} = 0,\tau)$ by the form $e^{-\Delta_c\tau}$ with $\Delta_c \equiv E_0^{N+1} - E_0^N$ for *large* values of τ. Figure 1(b) shows Δ_c as a function of linear lattice size. The data points for lattice sizes ranging from 4×4 to 16×16 fit very well a $1/L$ form which we use to extrapolate to the thermodynamic limit to obtain $\Delta_c/t = 0.67 \pm 0.015$. This result stands in good agreement with the quoted result of Furukawa and Imada [17]: $\Delta_c/t = 0.58 \pm 0.08$. Since in the notation of Eq. (1) the Hubbard model satisfies particle-hole symmetry at $\mu = 0$, the critical chemical potential is nothing but the charge gap $\mu_c \equiv \Delta_c$.

For values of the chemical potential within the charge gap, $|\mu| < \mu_c$, the zero-temperature Green function is real and may be obtained through the relation

$$G(\vec{r},\omega = \mu) = -\int_{-\infty}^{\infty} d\tau G(\vec{r},\tau)e^{\tau\mu}. \quad (7)$$

The Green function $G(\vec{r},\tau)$ is computed at half-band filling, where the sign problem is not present and

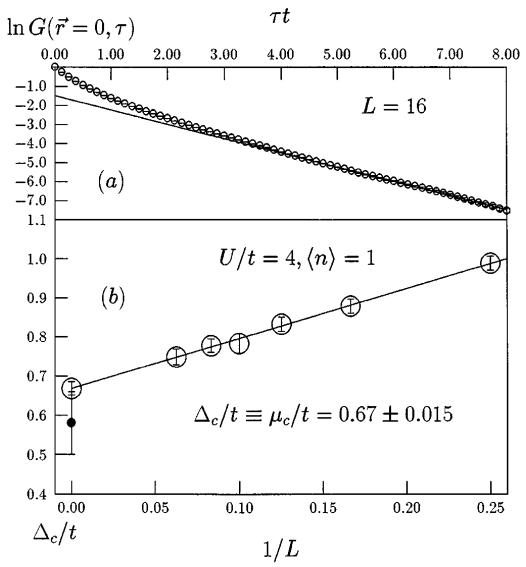

FIG. 1. (a) $\ln G(\vec{r} = 0,\tau)$ as a function of τ for the half-filled ($\mu = 0$) 2D Hubbard model at $U/t = 4$ on a 16×16 lattice. The solid line corresponds to a least square fit of $G(\vec{r} = 0,\tau)$ by the form $\exp(-\Delta_c\tau)$ at *large* values of τ. (b) Δ_c as a function of linear lattice size L. The solid circle at $1/L = 0$ corresponds to Δ_c as obtained in Ref. [17].

the statistical uncertainty does not grow exponentially with lattice size. However, since we are multiplying the QMC data by the factor $e^{\tau\mu}$, the statistical uncertainty will grow exponentially with increasing values of τ for $\tau\mu > 0$. For each lattice size L, we have considered the largest distance $\vec{r} = (L/2, L/2)$. For this distance, $G(\vec{r} = (L/2, L/2), \tau)$ is plotted in Fig. 2. Because of particle-hole symmetry at $\mu = 0$, $G(\vec{r} = (L/2, L/2), \tau) = -G(\vec{r} = (L/2, L/2), -\tau)$. For the imaginary time integration [see Eq. (7)] and values of the chemical potential $|\mu| < 0.65t$, a cutoff of $\tau t = 10$ proved to be sufficient for the determination of the Green function (see Fig. 2). $G(\vec{r} = (L/2, L/2), \omega = \mu)$ as a function of lattice size is plotted in Fig. 3 for several values of μ. For lattice sizes ranging from $L = 6$ to $L = 16$, an exponential decay may be seen within the quoted statistical uncertainty. From these data, we obtain an estimate of the localization length ξ_l. With the above determined value of μ_c, we plot $|\mu - \mu_c|$ versus ξ_l (see Fig. 4) on a log-log plot. For all considered chemical potentials, $\xi_l/a < 8\sqrt{2}$ which corresponds to our largest considered distance ($L = 16$). The slopes in Fig. 4 correspond to values of the critical exponent $\nu = 1/2$ and $\nu = 1/4$. The QMC data are consistent with $\nu = 1/4$ and seem to rule out the possibility $\nu = 1/2$. A statistical analysis yields $\nu = 0.26 \pm 0.05$.

To confirm the validity of our approach, we consider the Mott transition in the 1D Hubbard model at $U/t = 4$. A similar QMC calculation as described above for the 2D case yields a value of the correlation length exponent consistent with $\nu = 1/2$ (see Fig. 5). We obtain $\mu_c/t = 0.66 \pm 0.015$, which is consistent with the exact result of Lieb and Wu [18]: $\mu_c/t = 0.643$. Chains of linear length up to $L = 24$ were considered.

An interpretation of our results may be obtained by assuming a hyperscaling form for the singular part of the free energy which leads to the scaling relations

$$\xi_l \sim \Delta^{-\nu}, \qquad \chi_c \sim \Delta^{-\nu(z-d)}, \qquad D \sim \Delta^{\nu(d+z-2)}, \tag{8}$$

where $\Delta = |\mu - \mu_c|$, d is the dimensionality, and ν (z) corresponds to the correlation length (dynamical) exponent [2]. Since the control parameter Δ corresponds to the chemical potential, one obtains the additional constraint $\nu z = 1$ as well as $\delta \sim \Delta^{\nu(d+z)-1}$, δ being the doping concentration. In this formulation, the generic band insulator in all dimensions, as well as the Mott transition in the 1D Hubbard model, are characterized by the exponents $\nu = 1/2$ and $z = 2$ [2,5–7]. This stands in agreement with our QMC result, $\xi_l \sim |\mu - \mu_c|^{-1/2}$, for the 1D Hubbard model. In the 2D case we may combine our result in the insulating phase, $\xi_l \sim |\mu - \mu_c|^{-1/4}$, with the compressibility data of Furukawa and Imada [17] in the metallic phase, $\chi_c \sim |\mu - \mu_c|^{-1/2}$, to see that the above scaling relations are satisfied provided that $\nu = 1/4$ and $z = 4$. We note that our result for the 2D case has the following consequences. On one hand, it shows that mean-field descriptions of the Mott transition in the 2D case (e.g., the Hartree-Fock approximation, mean-field approximations of slave bosons, etc.) are inadequate since

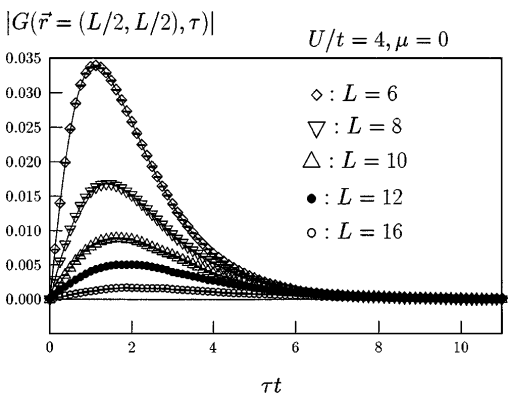

FIG. 2. $|G(\vec{r} = (L/2, L/2), \tau)|$ as a function of system size and imaginary time τ for the 2D Hubbard model.

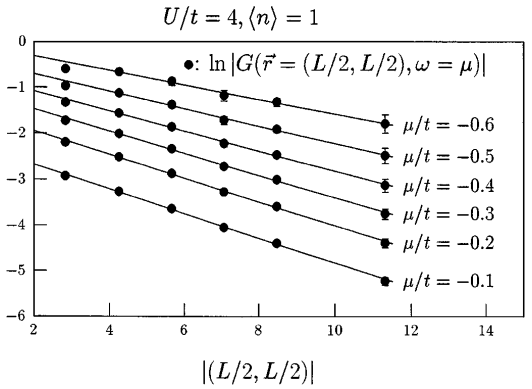

FIG. 3. $\ln|G(\vec{r} = (L/2, L/2), \omega = \mu)|$ as a function of distance and chemical potential for the 2D Hubbard model. The solid lines correspond to a least square fit of $|G(\vec{r} = (L/2, L/2), \omega = \mu)|$ by the form $\exp(-|\vec{r}|/\xi_l)$ for $L > 4$.

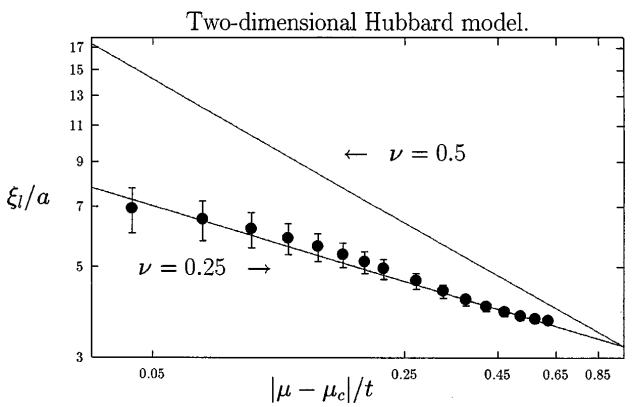

FIG. 4. Localization length ξ_l versus $|\mu - \mu_c|$ for the 2D Hubbard model. The solid lines correspond to two values of the correlation length exponent $\nu = 1/4$ and $\nu = 1/2$. The solid circles correspond to the QMC data.

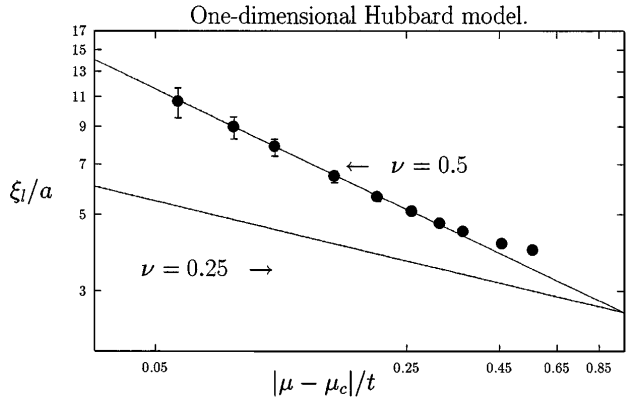

FIG. 5. Same as Fig. 4 but for the 1D Hubbard model.

they yield $\xi_l \sim |\mu - \mu_c|^{-1/2}$. On the other hand, it shows that the critical behavior of the Mott transition in the 1D and 2D Hubbard models differ since, in the 1D case, our result is consistent with $\xi_l \sim |\mu - \mu_c|^{-1/2}$. Both above points do not necessarily follow from the compressibility data of Furukawa and Imada [17].

In conclusion, we have determined the correlation length exponent from the knowledge of ξ_l in the insulating phase of the 2D Hubbard model and obtained $\nu = 0.26 \pm 0.05$. We have shown that a similar calculation for the 1D Hubbard model yields results consistent with $\nu = 1/2$. Our results show that the Mott transition in the 2D Hubbard model belongs to a new universality class, consistent with the assumption of hyperscaling and characterized by the exponents $\nu = 1/4$ and $z = 4$. Several anomalous aspects of the MIT are inferred when it is characterized by this new universality class [2]. Based on a single-particle theory, the exponents $\nu = 1/4$, $z = 4$ are consistent with the interpretation of the Mott transition driven by the divergence of the effective mass as opposed to the vanishing of the number of charge carriers. This statement is supported by the compressibility in the metallic phase [17] as well as by the high frequency Hall coefficient [19]. Another consequence of the exponent $\nu = 1/4$ is the behavior of the Drude weight in the vicinity of the Mott transition: $D \sim \delta^2$, δ being the hole density. As a byproduct, we have produced an accurate estimate of the charge gap for the 2D Hubbard model at $U/t = 4$: $\Delta_c/t = 0.67 \pm 0.015$. From the technical point of view, we have introduced an efficient method to obtain information on the nature of the MIT by approaching the transition from the insulator side. The most important fact is that for models which show particle-hole symmetry, such as dimerized Hubbard models, the method presented here is not plagued by the sign problem, and large lattice sizes may be considered.

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[1] W. Kohn, Phys. Rev. **133**, A171 (1964).
[2] M. Imada, J. Phys. Soc. Jpn. **64**, 2954 (1995).
[3] We define the zero-temperature Green function by $iG(\vec{r}, \omega) = \sum_\sigma \int dt e^{i\omega t} \langle \Psi_0 | T c_{\sigma,\vec{r}}(t) c^\dagger_{\sigma,\vec{0}}(0) | \Psi_0 \rangle$. Here, the notation is standard [10], and $|\Psi_0\rangle$ corresponds to the ground state in the insulating phase.
[4] F. F. Assaad and M. Imada, J. Phys. Soc. Jpn. **65**, 189 (1996).
[5] M. Imada, J. Phys. Soc. Jpn. **63**, 3059 (1994).
[6] T. Usuki, N. Kawakami, and A. Okiji, Phys. Lett. A **135**, 476 (1989).
[7] B. S. Shastry and B. Sutherland, Phys. Rev. Lett. **65**, 243 (1990).
[8] For the dispersion relation $\epsilon_{\vec{k}} = \vec{k}^2/2m$ the integration may be done analytically to obtain the result $\xi_l \sim |\mu - \mu_c|^{-1/2}$, with $\mu_c = 0$.
[9] P. W. Anderson, Phys. Rev. **124**, 41 (1961).
[10] G. D. Mahan, *Many-Particle Physics* (Plenum Press, New York, 1981).
[11] D. C. Herbert and R. Jones, J. Phys. C **4**, 1145 (1971).
[12] A. MacKinnon and B. Kramer, Phys. Rev. Lett. **21**, 1546 (1981).
[13] S. Sorella, S. Baroni, R. Car, and M. Parrinello, Europhys. Lett. **8**, 663 (1989); S. Sorella, E. Tosatti, S. Baroni, R. Car, and M. Parrinello, Int. J. Mod. Phys. B **1**, 993 (1989).
[14] G. Sugiyama and S. E. Koonin, Anal. Phys. **168**, 1 (1986).
[15] J. J. Deisz, W. von der Linden, R. Preuss, and W. Hanke, in "Computer simulations in Condensed Matter Physics VIII," edited by D. P. Landau, K. K. Mon, and H. B. Schüttler (Spinger-Verlag, Heidelberg, Berlin, to be published).
[16] S. R. White *et al.,* Phys. Rev. B **40**, 506 (1989).
[17] N. Furukawa and M. Imada, J. Phys. Soc. Jpn. **62**, 2557 (1993).
[18] E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).
[19] F. F. Assaad and M. Imada, Phys. Rev. Lett. **74**, 3872 (1995).