Critical Exponents of the Metal-Insulator Transition in the Two-Dimensional Hubbard Model.

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We study the filling-controlled metal-insulator transition in the two-dimensional Hubbard model near half-filling with the use of zero temperature quantum Monte Carlo methods. In the metallic phase, the compressibility behaves as 
\[ \kappa \propto |\mu - \mu_c|^{-0.58 \pm 0.08} \]
where \( \mu_c \) is the critical chemical potential. In the insulating phase, the localization length follows 
\[ \xi_l \propto |\mu - \mu_c|^{-\nu_l} \] with \( \nu_l = 0.26 \pm 0.05 \). Under the assumption of hyperscaling, the compressibility data leads to a correlation length exponent \( \nu_\kappa = 0.21 \pm 0.04 \).

Our results show that the exponents \( \nu_\kappa \) and \( \nu_l \) agree within statistical uncertainty. This confirms the assumption of hyperscaling with correlation length exponent \( \nu = 1/4 \) and dynamical exponent \( z = 4 \). In contrast the metal-insulator transition in the generic band insulators in all dimensions as well as in the one-dimensional Hubbard model satisfy the hyperscaling assumption with exponents \( \nu = 1/2 \) and \( z = 2 \).

KEYWORDS: metal-insulator transition, Hubbard model, hyperscaling, quantum critical phenomena

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Physics of the metal-insulator (M-I) transition has been studied over decades from the point of view of quantum critical phenomena and strong correlation effects. Recently, an approach to the M-I transition using a hyperscaling hypothesis has been developed by one of the authors (M.I). Let us consider the filling-controlled M-I transition in the ground state, which is controlled by the shift of the chemical potential

$$\Delta = \mu - \mu_c.$$  

(1)

Here $\mu$ is the chemical potential while $\mu_c$ is its critical value at the M-I transition. If we assume the single parameter scaling hypothesis, the correlation length of the system $\xi$ is described as

$$\xi \sim |\Delta|^{-\nu},$$  

(2)

and the singular part of the free energy is given by

$$f_s(\Delta) \sim |\Delta|^{\nu(d+z)}.$$  

(3)

Here, $z$ is the dynamical exponent, while $d$ is the dimensionality of the system. In the metallic phase, the doping concentration $\delta \equiv 1 - n$ near the phase transition is given by

$$\delta \sim \frac{\partial f_s}{\partial \mu},$$  

(4)

so that from eq. (3) we have

$$\delta \sim |\Delta|^{\nu(d+z)-1} = |\Delta|^{\nu d}.$$  

(5)

Here we used the relation $\nu z = 1$ which is obtained from the generalized Josephson relation.

In the case of the Hubbard model on a square lattice near half-filling, it has been shown by two of the authors (N.F. and M.I.) (hereafter NF-MI) that $\delta$ satisfies

$$|\Delta| \propto \delta^2.$$  

(6)

This result was obtained by computing the chemical potential,

$$\mu = -\frac{\partial E_G}{\partial \delta}$$  

(7)

at $U/t = 4$ on $4 \times 4$ to $12 \times 12$ lattices, in the standard notations. Here $E_G$ denotes the ground state energy. The calculations were carried out with the zero-temperature quantum Monte Carlo algorithm. This result implies that the compressibility diverges as

$$\kappa \equiv \frac{\partial \delta}{\partial \mu} \sim |\Delta|^{-1/2},$$  

(8)

when we approach the M-I transition from the metallic side. However, in NF-MI, an estimate of the statistical error of the exponent was not done, mainly due to large statistical uncertainty in location of the critical point, $\mu_c$. 


Recently, two of the authors (F.F.A. and M.I.) have computed with QMC methods, zero temperature imaginary time displaced Green function in the insulating phase. From this data they obtain an accurate estimate of the critical chemical potential at $U/t = 4$: $\mu_c = 0.67 \pm 0.05$ in units of the hopping matrix element. This result is obtained by extrapolating to the thermodynamic limit from data on $4 \times 4$ to $16 \times 16$ lattice.

Combining this value with the chemical potential data of NF-MI in the metallic phase leads to:

$$|\Delta| \propto \delta^{2.38 \pm 0.43}$$

(see Fig. 1). From this result and the assumption of hyperscaling we obtain a value of the correlation length exponent

$$\nu_\kappa = 0.21 \pm 0.04.$$ 

(10)

Fig. 1. Log-log plot of $|\mu - \mu_c|/t$ verses $\delta$ in the metallic phase. Here, $\mu_c/t = 0.67 \pm 0.05$. The line is the least-squares fit to the data.
In order to directly determine the correlation length exponent, FF A-MI\(^7\) have computed the Green function \(G(\mathbf{r}, \omega = \mu)\) for values of the chemical potential within the charge gap. For those values of the chemical potential, \(G(\mathbf{r}, \omega = \mu) \propto e^{-|\mathbf{r}|/\xi_l}\). The localization length, \(\xi_l\), diverges as the M-I transition is approached from the insulating side. We obtain numerically:

\[
\xi_l \propto |\Delta|^{-0.26 \pm 0.05}
\]  
(11)

(see Fig. 2). From this result, we obtain an estimate of the correlation length exponent:

\[
\nu_l = 0.26 \pm 0.05.
\]  
(12)

![Log-log plot of |\(\mu - \mu_c\)|/t versus \(\xi_l\) in the insulating phase. Here, \(\mu_c/t = 0.67 \pm 0.05\). The line is the least-squares fit to the data.](image)

Fig. 2. Log-log plot of \(|\mu - \mu_c|/t\) verses \(\xi_l\) in the insulating phase. Here, \(\mu_c/t = 0.67 \pm 0.05\). The line is the least-squares fit to the data.

If hyperscaling is valid, one expects the relation:

\[
\nu_\kappa \equiv \nu_l.
\]  
(13)

That the exponents should be equal on either side of the critical point is obtained through the scaling properties, and from the fact that the insulating and metallic phases may be
connected smoothly around the critical point $\Delta = 0$. The main result of this paper is that eq. (13) is satisfied within statistical uncertainty, thus putting on a firm numerical basis the assumption of hyperscaling. The M-I transition in 2D Hubbard model belongs to the universality class characterized by $\nu = 1/4$ and $z = 4$. This stands in contrast to the generic band M-I transition in all dimensions as well as to the Mott transition in the 1D Hubbard model, which both belong to the universality class $\nu = 1/2$ and $z = 2$. The M-I transition in 2D Hubbard model belongs to the universality class characterized by $\nu = 1/4$ and $z = 4$. This stands in contrast to the generic band M-I transition in all dimensions as well as to the Mott transition in the 1D Hubbard model, which both belong to the universality class $\nu = 1/2$ and $z = 2$.

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[8] We introduce small but finite staggered magnetic field $h_s$ and temperature $T$. With this construction, $f_s$ in the insulating and metallic phases may be connected smoothly along a path in the $\Delta, h_s$, and $T$ space. This leads to the equality of the exponents $\nu_l = \nu_s$.
[9] Recently, the exponent $\nu_s$ has also been estimated from the finite size scaling of Yang-Lee zeros at finite temperature, in E. Abraham, I.M. Barbour, P.H. Cullen, E.G. Klepfish, E.R. Pike and S. Sarkar: Phys. Rev. B53 (1996) 7704. Their result shows a critical behavior with $\nu_s = \frac{1}{4} \pm \frac{1}{6}$, which is consistent with our results. They interpret the result as a sign of the phase transition at finite temperature. However, the coincidence of the exponent $\nu_s$ with our zero temperature calculation suggests that their calculation has been performed in the quantum critical regime near the transition point. Therefore, we consider that their result also indicates that $\nu = 1/4$ and $z = 4$ at zero temperature.
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