Finite Temperature Mott Transition in the Hubbard Model in Infinite Dimensions

Marcelo J. Rozenberg

Departamento de Física, FCEN, Universidad de Buenos Aires, Ciudad Universitaria Pabellón I, 1428 Buenos Aires, Argentina

R. Chitra and Gabriel Kotliar

Serin Physics Laboratory, Rutgers University, Piscataway, New Jersey 08854

(Received 7 May 1999)

We study the second order finite temperature Mott transition point in the fully frustrated Hubbard model at half filling, within dynamical mean field theory. Using quantum Monte Carlo simulations and analytical arguments, we show the existence of a finite temperature second order critical point by explicitly demonstrating the existence of a divergent susceptibility as well as by finding coexistence in the low temperature phase. We determine the precise location of the finite temperature Mott critical point in the (U, T) plane. Our study verifies and quantifies a scenario for the Mott transition proposed in earlier studies of this problem.

PACS numbers: 71.30.+h, 71.27.+a

When the ratio of the strength of the electron-electron interaction to the bandwidth is increased, a metal insulator transition (MIT) occurs [1]. This phenomenon has been continuously and intensively studied in narrow bandwidth systems for several decades [2], with V_2O_3 being the archetypal system.

Providing a detailed theoretical description of this transition in systems which are not magnetically ordered is one of the most challenging problems in condensed matter physics. In recent years, great progress was achieved using the dynamical mean field theory (DMFT), a method which becomes exact in the limit of large lattice coordination. Within this framework, one can describe both metallic and insulating phases. See [3] for a review. Though some aspects of this theory agree with the scenarios put forth earlier by Brinkman and Rice and by Hubbard [4,5], the DMFT approach suggested important qualitative modifications of these pictures.

At zero temperature, in the DMFT of the fully frustrated Hubbard model, upon increasing the interaction the paramagnetic metallic state is destroyed at a critical value denoted by U_{c2} [6]. On the other hand, the insulating solution that exists for large U disappears when U is decreased, at a different critical value U_{c1}, at which the gap closes. Since $U_{c1} < U_{c2}$, there is a region where two phases, i.e., a paramagnetic metal and a paramagnetic insulator, coexist. This region of coexistence naturally extends to finite temperatures, where it is bounded by two lines $U_{c1}(T)$ and $U_{c2}(T)$. Consequently, at finite temperatures, a *first order* metal to insulator transition takes place at a value of the interaction $U_c(T)$, with $U_{c1}(T) < U_c(T) < U_{c2}(T)$ [7,8].

At temperatures above this transition line, two different crossover regions were identified [6,9]. The first crossover region is the natural continuation of the $U_{c2}(T)$ line, and was characterized as the place where the low energy resonance in the spectral function rapidly loses its intensity and the resistivity increases rapidly. The second crossover region can be considered to be the natural extension of the $U_{c1}(T)$, and was characterized as the line where the gap is comparable to the temperature and where a crossover to activated behavior in the resistivity is seen. These crossover lines were further related [9] to the experimental observations of McWhan *et al.* and Kuwamoto *et al.* [10,11]. Note that generically within DMFT, i.e., both at high and low temperatures, the destruction of the metallicity and the gap closure occur at different locations on the phase diagram. The only exception to this is the finite temperature second order critical point at which the two boundary lines $U_{c1}(T)$ and $U_{c2}(T)$ meet and terminate. In this paper, we provide a description of this second order point at which the MIT occurs.

Though substantial evidence indicated [3] that the qualitative aspects of the finite temperature MIT that is described above were genuine properties of the exact solution of the model, recent quantum Monte Carlo (QMC) work challenged this scenario [12]. In Ref. [12] it was claimed that, within the temperature range numerically accessible to the QMC technique, it was not possible to find any evidence for a *finite temperature* MIT point. It is very important to clarify this issue, since our earlier work has successfully predicted new experiments in V_2O_3 [9] and provided a natural interpretation of earlier data [10,11]. We describe below how the MIT point can be found, and we determine its location with reasonable accuracy, illustrating the power but at the same time the subtleties of the QMC technique when applied in conjunction with the self-consistent DMFT equations.

Besides quelling the doubts raised recently in Ref. [12], there are other motivations for this work. As stressed by Nozières [13], the Mott transition lacks an obvious order parameter, so it is not clear *a priori* which quantities should exhibit singular behavior. Second, the second

 0031-9007/99/83(17)/3498(4)$15.00

order Mott end point is observed experimentally in V_2O_3 and $NiSe_xS_{2-x}$, and its properties are the subject of ongoing experiments. Finally, it is important from the point of view of numerical studies of correlated electron systems. Since a full analytic solution to this problem is unavailable, the understanding of models in the limit of large lattice coordination requires numerical work and analytic approximations. This is a common situation in the field of correlated electron systems, and the Hubbard model in infinite dimensions provides an excellent playground to test the merit of various analytic approximations and numerical methods.

We consider the Hubbard model on the Bethe lattice in the paramagnetic phase [14] with coordination d and hopping $t/\sqrt{d}$ in the $d \to \infty$ limit [15] at half filling:

$$H = -\sum_{\langle i,j\rangle\sigma\omega} \frac{t}{\sqrt{d}} (c_{i\sigma}^{+} c_{j\sigma} + \text{c.c.}) + \sum_i U n_{i\uparrow} n_{i\downarrow} . \quad (1)$$

The half bandwidth is given by $D = 2t$ and we set $D = 1$ as a unit of energy. The chemical potential is set equal to $\frac{U}{2}$ at half filling.

All the *local* correlation functions can be obtained from a single impurity Anderson model (SIAM) with a hybridization function,

$$\Delta(i\omega_n) = \sum_k \frac{V_k^2}{i\omega_n - \epsilon_k} , \quad (2)$$

provided that $\Delta(i\omega_n)$ obeys the self-consistency condition [16]:

$$t^2 G_{\text{imp}}(i\omega_n)[\Delta, \alpha] = \Delta(i\omega_n) . \quad (3)$$

Here, α denotes the control parameters of the problem U and T. $G_{\text{imp}}(i\omega_n)[\Delta]$ is the finite temperature Matsubara f-electron Green's function of the SIAM:

$$H_{\text{SIAM}} = \sum_{k\sigma} \epsilon_k c_{k\sigma}^{+} c_{k\sigma} + V_k (c_{k\sigma}^{+} f_\sigma + f_\sigma^{+} c_{k\sigma}) + U n_{f\uparrow} n_{f\downarrow} . \quad (4)$$

To solve the problem, the single impurity Green's function is calculated using QMC or exact diagonalization methods and (3) is used to check for self-consistency [3]. This iterative process is continued until self consistency is achieved. At that point, $G_{\text{imp}}(i\omega_n)$ coincides with $G_{\text{loc}}(i\omega_n)$, the *local* Green's function of the original *lattice* problem. At each iteration step we use quantum Monte Carlo simulations [17] to calculate the impurity Green's function in imaginary time [18]. This algorithm is widely considered to provide numerically exact solutions to the model (in the Monte Carlo sense).

The parameters of the simulation are as follows: we typically perform 60 000 sweeps (1 sweep = 1 attempt to update each of the L pseudospins = L attempts, where L is the number of time slices used), and, when required, up to 300 000 sweeps in order to minimize the enhanced fluctuations close to the critical point. We always set the length of the time slice $\Delta\tau = \beta/L \leq 0.5$, where β is the inverse temperature.

As a criterion for the convergence of the numerical solution of the DMFT equations, we monitor the evolution with the iteration number of $G(i\omega_1)$, the value of the Green's function at the first Matsubara frequency. This quantity is appropriate, as it is essentially the integral of $G(\tau)$ (with τ being the imaginary time), the quantity that is directly computed statistically in the QMC calculation. Also, $G(i\omega_1)$ is the value of the frequency dependent Green's function that fluctuates most; thus, it sets an upper bound for the statistical error of the whole $G(i\omega_n)$. We stop the iterations when the fluctuations in $G(i\omega_1)$ become of the order of the statistical error of the QMC (which is controlled by the number of sweeps at a given U and T) and remain stable for at least about 30 more iterations.

In generic regions of the (U, T) plane, less than 10 iterations are sufficient to obtain a converged solution. However, since we are looking for a critical point which is a bifurcation point of (3), the number of iterations needed to obtain convergence diverges, as we approach the critical point. This is the usual phenomenon of critical slowing down associated with bifurcating solutions in recursive procedures and it forces us to increase the number of iterations, as we approach the critical point. For example, up to 300 iterations were necessary to check the convergence at parameter values close to the critical point. Special care was taken to assure that the solutions were indeed converged. To this end, we used two different initial seeds for the iterative procedure: $G(\tau)[U = 0]$ that corresponds to a metallic state, and a $G(\tau)[t = 0]$ that corresponds to an insulating one. These two initial Green's functions have qualitative different behavior at low frequencies, one with a finite density of states at the Fermi energy and the other with an insulating gap. If there is a single solution to the mean field equations, the algorithm should in both cases evolve towards the unique attractor. If two different solutions are allowed, one metalliclike and one insulatorlike, it may be expected that the metallic seed would evolve towards the former and the insulating seed towards the latter. Using this method, when we find a converged unique solution to (3), we are certain that the algorithm has fully converged.

To prove the existence of a finite temperature critical point, we need to isolate a physical quantity that exhibits singular behavior. We view this MIT as a liquid gas transition, where the double occupancy $\langle d \rangle$ plays the role of the density, while U plays the role of the pressure and T the natural role of temperature. This analogy was put forward in an insightful paper by Castellani *et al.* [19]. As shown here, their scenario is realized within the DMFT solution of the Hubbard model. With this analogy to the liquid gas transition in mind, we focus on the behavior of the double occupation as a function of temperature and

interaction strength. We define the susceptibility $\chi = \max_U[\partial\langle d\rangle/\partial U]$ that, as we shall later show, is a quantity that diverges at the finite T second order critical point.

In Fig. 1, we show our results for the double occupation $\langle d\rangle$ as a function of U. Each set of data is obtained at a constant T, and we have checked the uniqueness of the solutions using the procedure described above.

The most remarkable feature is the rapid variation of $\langle d\rangle$ with the interaction U at the lower temperatures [8]. This variation is a direct consequence of a divergence in the susceptibility χ defined earlier. In order to obtain the susceptibility from the discrete set of data at each temperature, we fit the numerical results with analytic expressions that follow from a Ginzburg-Landau analysis [20] to be discussed elsewhere. We obtain the curve $\chi^{-1}(T)$ (which is plotted in the inset of Fig. 1) that can be approximated, close to the transition, with the expression $\chi^{-1} = \frac{t}{a+bt}$, where t is the reduced temperature $t = T - T_c$, and a and b are real positive parameters. More precisely, $\langle d\rangle(U,T)$ contains a singular part (arising from the liquid gas analogy close to the transition) and a regular part. The regular part gives the constant background (b/a) and the singular part produces the divergent susceptibility (a/t) which is linear in the inverse reduced temperature. T_c and U_c are fitting parameters, which give the location of the second order critical point where the first order lines terminate. A least squares fit to χ gives our estimate for $T_c = 0.026 \pm 0.003$ and using the liquid gas analogy we find that $U_c = 2.38 \pm 0.02$. Thus, we have obtained estimates for the position of the finite temperature second order critical point in the single band Hubbard model using the QMC method [21]. It is important to realize now that the lowest temperature set of data for the double occupation in Fig. 1 at $T = 1/40 = 0.025$ appears to be slightly *below* T_c. These results thus indicate a *discontinuous* jump in the double occupation.

A more general consequence of the presence of the finite temperature second order critical point is the existence of a region at T lower than T_c, where two different solutions of the mean field equations exist. This coexistence of solutions, as usual, results in first order transition lines. We have, therefore, searched for different converged solutions well below $T_c = 0.026$ and performed calculations at $T = 1/51.2$ and $T = 1/64$ for several values of U close to U_c. Indeed, we obtained two different and fully converged solutions at $U = 2.4$ in the first case, and at $U = 2.4$ and $U = 2.5$ in the latter. For the $U = 2.4$ and $T = 1/64$ solutions, we have taken special care to rule out the possibility of systematic errors, by performing a large number of further iterations after self-consistency was achieved and also by increasing the number of sweeps to up to 300 000 to minimize statistical fluctuations. In Fig. 2, we display two coexistent solutions at $U = 2.4$ and $T = 1/64$, along with the results for the imaginary part of the Green's functions on the real frequency axis using the maximal entropy method [22] for the analytic continuation. These results, obtained within a narrow range of interaction U close to U_c and at temperatures *below* our estimate for T_c, further confirm the consistency of our numerical results.

In conclusion, we presented the results of a careful numerical QMC study of the finite temperature Mott transition in the paramagnetic phase of the Hubbard model in infinite dimensions. We identified the singular behavior of a susceptibility associated with the finite temperature critical point, and reasonably accurate estimates for U_c and T_c were obtained. This should be contrasted with a previous QMC study of the same problem [12] which reached the conclusion that there is no signature of a finite

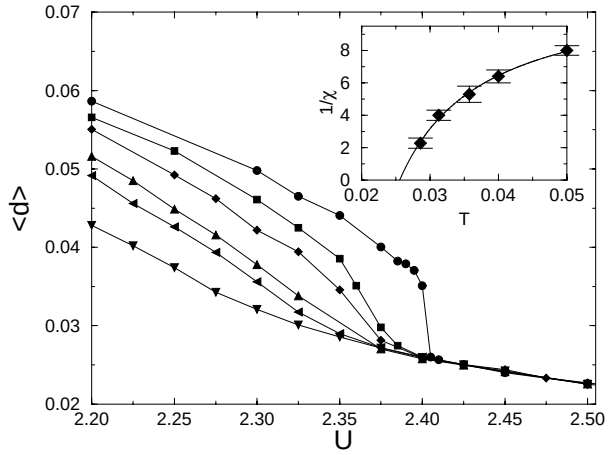

FIG. 1. The double occupation $\langle d\rangle$ as a function of U for several values of $T = 1/20$, $1/25$, $1/28$, $1/32$, $1/35$, and $1/40$ (from bottom to top). The inset shows the inverse susceptibility χ^{-1} as a function of T. The line is a least squares fit using the expression in the text. The intercept with the T axis gives our estimate for $T_c = 0.026$.

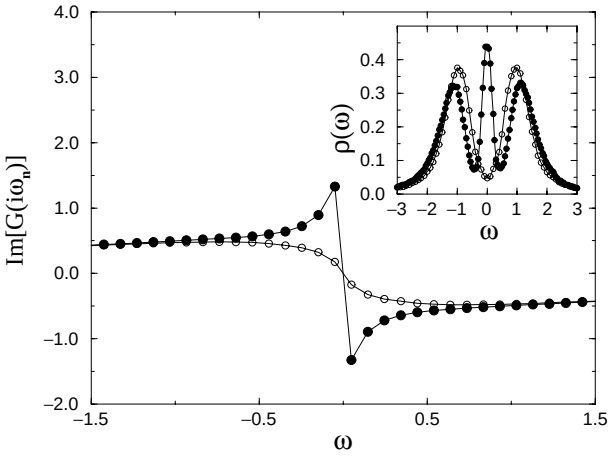

FIG. 2. Two converged solutions, one metalliclike (solid circles) and one insulatinglike (open circles), of the DMFT equations for the same value of the interaction $U = 2.4$ and $T = 1/64$. In the inset we show their corresponding densities of states.

temperature second order phase transition in the temperature region accessible to QMC studies. Furthermore, they presented $T_{\text{bound}} = 0.014\,29$ as a rigorous numerical upper bound on T_c. Here we have shown using two different approaches, i.e., a high temperature susceptibility calculation and an explicit demonstration of coexistence at low temperatures, that a finite temperature critical point exists and that the bound obtained in [12] is incorrect.

In earlier publications we asserted that qualitative features of the paramagnetic metal to paramagnetic insulator transition observed in V_2O_3 are well described by the DMFT of the single band Hubbard model on a frustrated lattice treated using the iterated perturbation theory. In this work we show that those conclusions are also valid when a more accurate technique, such as QMC, is used to solve the dynamical mean field equations. In particular, the anomalous temperature dependence of physical properties (double occupancy, resistivity, etc.) and the crossovers discussed in Ref. [9], which were tied to the proximity to a second order finite temperature metal to insulator transition in the model.

While the qualitative agreement between the DMFT and the experiments is remarkable, there are quantitative disagreements. The measured plasma frequency is a factor of 2 larger than the calculated one (using exact diagonalization and DMFT), if we take the local density approximation (LDA) estimate of the bandwidth $D \approx 0.5$ eV [23]. This was already noticed in Refs. [9,24]. Using the same LDA based estimates for the model parameters, the critical temperature that we compute (with DMFT and QMC) is also approximately a factor of 2 smaller than the observed T_c in V_2O_3 [10].

These results suggest the necessity for the inclusion of additional features, such as orbital degeneracy, ligand bands [25], and the electron-phonon interaction [26] in the model, to be able to make accurate predictions for physical quantities in this system. The extension of the QMC algorithm to the orbitally degenerate models proposed by one of us [27] should be useful for this purpose. Indeed, less extensive studies than those carried out here suggest that orbital degeneracy increases substantially the critical temperature [27].

Useful conversations with G. Moeller and W. Krauth are acknowledged. This work was supported by NSF 95-29138. M. J. R. acknowledges support of Fundación Antorchas, CONICET (PID No. 4547/96), and ANPCYT (PMT-PICT1855).

[1] N. F. Mott, *Metal Insulator Transitions* (Taylor & Francis, London, 1974).
[2] For a review, see M. Imada, A. Fushimori, and Y. Tokura, Rev. Mod. Phys. **70**, 1039 (1998).
[3] For a review, see A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).
[4] J. Hubbard, Proc. R. Soc. London A **281**, 401 (1964).
[5] W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 4302 (1970).
[6] See Fig. 33 and Fig. 43 of Ref. [3] for the results obtained with the iterated perturbation theory approximation.
[7] X. Y. Zhang, M. J. Rozenberg, and G. Kotliar, Phys. Rev. Lett. **70**, 1666 (1993).
[8] A. Georges and W. Krauth, Phys. Rev. B **48**, 7167 (1993); M. J. Rozenberg, G. Kotliar, and X. Y. Zhang, Phys. Rev. B **49**, 10 181 (1994).
[9] M. J. Rozenberg, G. Kotliar, H. Kajueter, G. A. Thomas, D. H. Rapkine, J. M. Honig, and P. Metcalf, Phys. Rev. Lett. **75**, 105 (1995).
[10] D. McWhan *et al.*, Phys. Rev. B **7**, 3079 (1973).
[11] H. Kuwamoto, J. M. Honig, and J. Appel, Phys. Rev. B **22**, 2626 (1980).
[12] J. Schlipf, M. Jarrell, P. G. J. van Dongen, N. Blumer, S. Kehrein, Th. Pruschke, and D. Vollhardt, cond-mat/9902267.
[13] P. Nozières, Eur. Phys. J. B **6**, 447 (1998).
[14] As discussed in Ref. [1], these results become exact in many magnetically frustrated lattices which share the same density of states as the Bethe lattice in the limit of infinite coordination.
[15] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989).
[16] A. Georges and G. Kotliar, Phys. Rev. B **45**, 6479 (1992); see also Ref. [18].
[17] J. Hirsch and R. Fye, Phys. Rev. Lett. **56**, 2521 (1986).
[18] M. Jarrell, Phys. Rev. Lett. **69**, 168 (1992); M. J. Rozenberg, X. Y. Zhang, and G. Kotliar, Phys. Rev. Lett. **69**, 1236 (1992); A. Georges and W. Krauth, Phys. Rev. Lett. **69**, 1240 (1992).
[19] C. Castellani, C. Di Castro, D. Feinberg, and J. Ranninger, Phys. Rev. Lett. **43**, 1957 (1979).
[20] G. Kotliar, cond-mat/9903188.
[21] These estimates are very close to that obtained using the finite temperature exact diagonalization method with up to six sites ($U_c = 2.4, T_c = 0.024$); G. Moeller, Ph.D. thesis, Rutgers University, 1994.
[22] M. Jarrell and J. E. Gubernatis, Phys. Rep. **269**, 133 (1996).
[23] L. F. Mattheiss, J. Phys. Condens. Matter **6**, 6477 (1994).
[24] M. J. Rozenberg, G. Kotliar, and H. Kajueter, Phys. Rev. B **54**, 8452 (1996).
[25] T. Wolenski, M. Grodzicki, and J. Appel, cond-mat/9811095.
[26] P. Majumdar and H. R. Krishnamurthy, Phys. Rev. Lett. **73**, 1525 (1994).
[27] M. J. Rozenberg, Phys. Rev. B **55**, RC4855 (1997).