Coexistence of solutions in dynamical mean-field theory of the Mott transition

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(Received 16 August 1999)

In this paper, I discuss the finite-temperature metal-insulator transition of the paramagnetic Hubbard model within dynamical mean-field theory. I show that coexisting solutions, the hallmark of such a transition, can be obtained in a consistent way both from quantum Monte Carlo (QMC) simulations and from the exact diagonalization method. I pay special attention to discretization errors within the QMC method. These errors explain why it is difficult to obtain the solutions from the QMC method close to the boundaries of the coexistence region.

The Mott-Hubbard metal-insulator transition is one of the fundamental problems in the field of correlated electronic systems. During the last few years, dynamical mean-field theory (DMFT)[1,2] has emerged as an appropriate paradigm for this transition. Within DMFT, the paramagnetic half-filled Hubbard model on the Bethe lattice was found to undergo a first-order phase transition at finite temperature $T=1/\beta$. The hallmark of such a transition is the coexistence of two solutions for the same value of the electronic interaction U, with $U_{c_1}(\beta)<U<U_{c_2}(\beta)$. As is usual, I will label as ''insulating'' the solution which can be continuously followed at low temperature from large values of the interaction down to U_{c_1}, and as ''metallic'' the one which exists from $U=0$ up to U_{c_2}.

Recent work[3] has challenged the above scenario. Using the quantum Monte Carlo (QMC) method, rather than the exact diagonalization (ED) approach,[4] the authors of Ref. 3 were unable to detect coexistence in the DMFT equations. This is surprising, as the two algorithms had extensively been compared to each other (cf, e.g., Ref. 2 Sec. VI, Appendix C). The aim of the present paper is to discuss the conflicting numerical approaches (for related work, cf. Ref. 5). I show that coexisting metallic and insulating solutions can indeed be obtained using both methods in a transparent and completely consistent way. I pay special attention to the problem of discretization errors. It will become clear that the QMC method needs to use very fine discretizations in order to obtain the insulating solution close to U_{c_1}. Inside the coexistence region, the problem disappears. All the numerical work in this paper relies on programs which are publicly available.[2]

Given the large number of papers already published on the subject, I will not repeat the standard definitions for the half-filled Hubbard model on the Bethe lattice within DMFT. These can be found, e.g., in Ref. 2. The important parameter of the model is the bandwidth D (cf. Ref. 2); I quote interactions and temperatures in units of the bandwidth $D/\sqrt{2}$.

The point of departure of the present paper is Ref. 6, where coexisting solutions of the mean-field equations at inverse temperature $\beta D/\sqrt{2}=100$ were found (within ED) for $U_{c_1}<U<U_{c_2}$ with $U_{c_1}(\beta D/\sqrt{2}=100)\sim 3.3D/\sqrt{2}$ and $U_{c_2}(\beta D/\sqrt{2}=100)=3.8D/\sqrt{2}$.

For this paper, as a reference point I choose the values $U=3.55D/\sqrt{2}$ and $\beta D/\sqrt{2}=100$. At this point, both metallic and insulating solutions can be found easily by ED.[7] These solutions are given by bath Green's functions $\mathcal{G}_0(\tau)$ and impurity model Green's functions $G(\tau)$ (cf. Ref. 2 for definitions).

As we are far within the coexistence region, both solutions correspond to the bottoms of deep basins of attraction. I have perturbed the metallic bath Green's function, $\mathcal{G}_0^{met}(\tau)$, as well as the insulating one, $\mathcal{G}_0^{ins}(\tau)$, and fallen back into corresponding solutions after a few iterations. This situation changes as we approach the boundary of the coexistence region. For smaller U, for example, the insulating solution becomes less and less attractive, until the basin of attraction vanishes at U_{c_1}. This scenario simply corresponds to the familiar free-energy landscape at a first-order transition.

Both ED and the QMC method discretize some component of the DMFT equations. In ED, the discretization parameter is the number n_s of *sites* of the quantum impurity model, while in the QMC approach the number L of *slices* appears, with $\Delta\tau=\beta/L$ (cf. Ref. 2). I have computed the insulating bath Green's function $\mathcal{G}_0^{ins}(\tau)$ at the reference point for $n_s=5,6$, and 7. Each of the solutions (for fixed n_s) is fully converged; in addition, the convergence with the number of sites n_s is excellent. I stress in passing that the sites in the ED algorithm are chosen in an optimal way, very similar to what is done in Gaussian integration.[8] Exponential convergence in n_s has been reported.[2] Given that $\mathcal{G}_0^{ins}(\tau,n_s=7)$ differs by less than 0.005 from $\mathcal{G}_0(\tau,n_s=6)$, I am led to the proposition that both $\mathcal{G}_0^{ins}(\tau,n_s=7)$ and $\mathcal{G}_0^{met}(\tau,n_s=7)$ are essentially exact. This assertion would have to be refuted for at least one of the solutions (in fact, for the insulating one) if we were to agree with the authors of Ref. 3.

The following reasoning will lead us to a very interesting result: consider a *single* iteration of the self-consistency loop starting from one of the solutions obtained with ED:

$$\mathcal{G}_0^{ins,met}\rightarrow G\rightarrow \mathcal{G}_0^{\rm new}. \tag{1}$$

If, contrary to our assertion, $\mathcal{G}_0^{ins}(\tau)$ or $\mathcal{G}_0^{met}(\tau)$ were not self-consistent, we should be able to detect differences, say, between $\mathcal{G}_0^{ins}$ and $\mathcal{G}_0^{\rm new}$ even by other methods than ED, for example by QMC simulation.

In this sense, I have discretized both $\mathcal{G}_0^{ins}$ and $\mathcal{G}_0^{met}$ (as obtained by ED) and used them as input for *single self-consistency loops* [as in Eq. (1)] of the QMC algorithm for

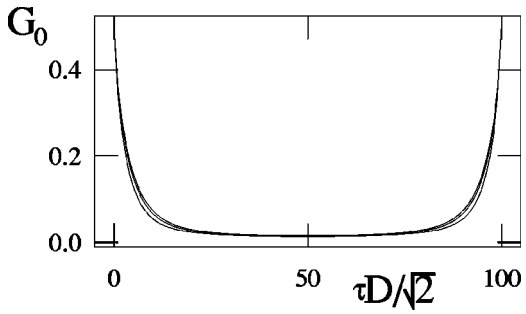

FIG. 1. $\mathcal{G}_0^{\rm new}(\tau,\Delta\tau)$ of the metallic solution, as computed by the QMC method for $\Delta\tau D/\sqrt{2}=1,0.5$ and $\mathcal{G}_0^{met}(\tau,n_s=7)$ (from below). Parameters of the reference point are $\beta D/\sqrt{2}=100$, and $U=3.55D/\sqrt{2}$.

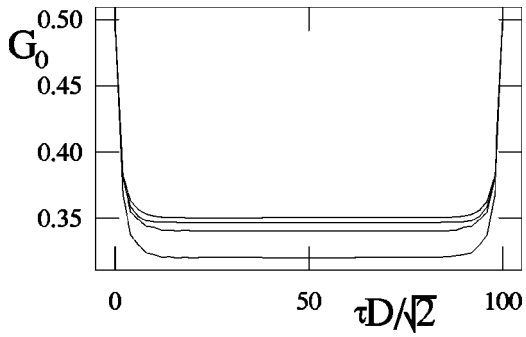

FIG. 2. $\mathcal{G}_0^{\rm new}(\tau,\Delta\tau)$ of the insulating solution, as computed by the QMC method for $\Delta\tau D/\sqrt{2}=1$, 0.5, and 0.25, and $\mathcal{G}_0^{ins}(\tau,n_s=7)$ (from below) at the reference point.

different values of $\Delta\tau$. From the discretized Green's function $G^{\Delta\tau}(\tau)$, we then compute $\mathcal{G}_0^{\rm new}(\tau)$ by inverse Fourier transformation. Results for the metallic solution are shown in Fig. 1. We see that the finite-$\Delta\tau$ effects are quite small. Clearly, $\mathcal{G}_0^{\rm new}(\tau,\Delta\tau)\to\mathcal{G}_0^{met}(\tau)$ as $\Delta\tau\to 0$. The metallic solution has not been contested.

The situation becomes much more illuminating as we consider the insulating solution $\mathcal{G}_0^{ins}(\tau)$, again as initial condition for a single QMC calculation to obtain $G^{\Delta\tau}$. In this case, I have computed $G^{\Delta\tau}(\tau)$ for $\Delta\tau=1,0.5$, and 0.25. The results for $\mathcal{G}_0^{\rm new}(\tau)$, again obtained by inverse Fourier transformation, are shown in Fig. 2: The upper curve shows $\mathcal{G}_0^{ins}(\tau,n_s=7)$, and the three lower curves represent $\mathcal{G}_0^{\rm new}(\tau)$ for $\Delta\tau D/\sqrt{2}=1,0.5$, and 0.25. It is evident that very large finite-$\Delta\tau$ effects are present. Note that *all* the curves $\mathcal{G}_0^{\rm new}(\tau,\Delta\tau)$ expose a plateau $\mathcal{G}_0\sim$const for τ away from 0 or β. Such a plateau is characteristic of an insulating solution (cf. Fig. 1), and its value *decreases* with the gap of the single-particle density of states. We thus arrive at the crucial observation that the finite-$\Delta\tau$ effects bias the self-consistency condition of the QMC algorithm toward the metallic solution. Nevertheless, we again find the ED solution as $\Delta\tau\to 0$. The data presented in Fig. 2 present a crucial consistency check of the two methods in the insulating phase.

In terms of the free-energy landscape mentioned earlier, this simply means that the picture at finite $\Delta\tau$ is *tilted*. The QMC iteration is dragged away from the insulating solution $\mathcal{G}_0^{ins}$ into the metal.

In addition to this effect, there seems to be no difference between the iteration loop of ED and the one of the QMC approach. Within a deep basin of attraction of the insulating solution, a small drag due to finite-$\Delta\tau$ effects should only lead to a shift of the solution, and its stability should be preserved. This is exactly what I have observed in independent simulations, which are analogous to what was done in Ref. 3. I ran *full* iteration loops starting from $\mathcal{G}_0^{ins}(\tau)$ for $\Delta\tau D/\sqrt{2}=1$ and $\Delta\tau D/\sqrt{2}=0.5$. In the first case, the simulation moved away from the insulation solution: After about ten iterations, the metallic solution was approximately recovered. In contrast, for $\Delta\tau D/\sqrt{2}=0.5$, the insulating solution is very clearly stable. A 40-day simulation of this single problem on a work station obtained a very well-converged self-consistent solution for $\mathcal{G}_0(\tau,\Delta\tau)$ within the QMC approach. This solution makes no more reference to ED, but it of course resembles the curves shown in Fig. 2; the plateau value is $\mathcal{G}_0(\tau D/\sqrt{2}=50)\sim 0.30$, comparable to the one-shot solution at the same value of $\Delta\tau$ (cf. Fig. 2).

In my opinion, the present discussion of the discretization errors and both the one-step iteration and the explicit self-consistent Monte Carlo solution leave little room but to accept the coexistence at finite temperature. It is evident that the Monte Carlo simulation at the insulating solution has important finite-$\Delta\tau$ effects. These errors modify the qualitative aspects of the solution only close to the phase boundaries where the basins of attraction of the insulating solution are shallow and small. Therefore, the discretization errors will be more pronounced close to U_{c_1}, and also at higher temperature.

It is a pleasure to thank G. Kotliar and A. Georges for helpful discussions.

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