Quantum Monte Carlo calculation of the finite temperature Mott-Hubbard transition

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We present clear numerical evidence for the coexistence of metallic and insulating dynamical mean field theory (DMFT) solutions in a half-filled single-band Hubbard model with bare semicircular density of states at finite temperatures. Quantum Monte Carlo (QMC) method is used to solve the DMFT equations. We discuss important technical aspects of the DMFT-QMC which need to be taken into account in order to obtain the reliable results near the coexistence region. Among them are the critical slowing down of the iterative solutions near phase boundaries, the convergence criteria for the DMFT iterations, the interpolation of the discretized Green’s function and the reduction of QMC statistical and systematic errors. Comparison of our results with those of other numerical methods is presented in a phase diagram.

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The Mott-Hubbard Transition is an outstanding open problem in condensed matter physics. The theoretical progress in this field has been impeded by non-perturbative nature of the strongly correlated system.

In recent years considerable progress has been made with a single band Hubbard model by using DMFT approximation which becomes exact in the limit of infinite coordinations (\( z = \infty \)). The most striking point of these works is a discontinuous metal-insulator transition (MIT) at finite temperature \( T \) which takes place at the critical interaction strength line \( U_c(T) \). This line lies inside a coexistence region where two phases, one metallic and one insulating coexist. The coexistence region is bounded by two lines \( U_{c1}(T) \) and \( U_{c2}(T) \) and \( U_{c1}(T) < U_c(T) < U_{c2}(T) \).

While this picture is now generally accepted by all groups working on the problem, the origin of the controversial results over the coexistence region in a single-band Hubbard model at finite temperature within QMC method, and more generally the difficulties in carrying out the DMFT-QMC algorithm have not been clarified. This is an important problem, since DMFT-QMC is currently being applied to many similar models with more complicated orbital and spin structure.

In this paper we provide clear evidence for the coexistence of metallic and insulating solutions in a half-filled single-band Hubbard model with bare semicircular density of states at finite temperature within DMFT-QMC calculation. We discuss several aspects of DMFT-QMC method which have to be taken into account in order to get the reliable results near a coexistence region. First, we identify the source of the main difficulties in running DMFT-QMC near the coexistence region: uncontrolled errors in DMFT-QMC in the region where critical slowing down is dominant. The critical slowing down of the DMFT iteration follows from the Landau analysis and can only be avoided by choosing a different rearrangement of the DMFT equation such as the one suggested by the Newton method. In this paper, however we use this critical slowing down as an indicator which allows us to locate boundaries of the coexistence region, and to fully confirm, using QMC methods, the predictions of the Landau analysis. We discuss how to minimize errors in DMFT-QMC calculation by using correct interpolation of the discretized Green’s functions in direct Fourier Transformation (FT) as well as a proper treatment of discontinuities of Green’s functions in inverse Fourier Transformation (iFT). Also extrapolation of data to the limit of \( \Delta \to 0 \) is used to reduce Trotter errors. Finally we obtain reliable coexistent insulating and metallic solutions within DMFT-QMC method and estimate the location of the first order MIT line \( U_c(T) \). In the limit of infinite dimensions a single-band Hubbard model is mapped onto an Anderson impurity model supplemented by a self-consistency condition. DMFT equation of this model,

\[
t^2G(i\omega)|\Delta| = \Delta(i\omega),
\]

is solved iteratively within QMC calculation, where \( \Delta(i\omega) \) and \( G(i\omega)|\Delta| \) are a hybridization function and a local Green’s function of the impurity model. Our energy unit is set to be \( t = 1/2 \) which comes from a scaled hopping amplitude, \( t/\sqrt{2} \), in an infinite dimensional single-band Hubbard model.

Within DMFT-QMC calculation, the coexistence region should be explored with a great care due to the following two reasons: critical slowing down and errors in DMFT-QMC. The critical slowing down is the critical phenomena which manifests itself by slowing down of the convergence rate of a numerical method. The critical slowing down at a phase boundary can be proved with the argument based on Landau free energy: no convergence at an inflection point of Landau free energy within iteration method. At a boundary of the coexistence region one solution never converges while another one converges fast. However around Mott endpoint (where \( U_{c1} \) and \( U_{c2} \) merge) both solutions converge slowly because the narrow coexistence region around Mott endpoint brings two boundaries close enough so as to make
a whole coexistence region numerically unstable as was pointed out in ref. [3]. Unless carefully taken care of, fluctuation of a solution originating from errors in DMFT-QMC may result in undesirable transition of one solution to another one in DMFT iteration around Mott endpoint where critical slowing down is dominant.

In this paper we show that one can use the existence of critical slowing down as an indicator of boundaries of the coexistence region. Near a coexistence boundary, $U_{c1}(T)$ or $U_{c2}(T)$, metallic and insulating solutions show different convergence patterns within DMFT iterations: one converges very slowly while the other converges in a few iterations. A convergence criterion is applied to determine required number of iterations to get a convergent solution. We locate the coexistence boundaries at which such iteration numbers diverge.

The convergence of a solution is determined by monitoring of the most fluctuating component $\text{Im} \Sigma(i\pi T)$, imaginary part of self energy at the first Matsubara frequency, as a function of number of iterations. QMC statistical error of $\text{Im} \Sigma(i\pi T)$ at each iteration is controlled by the number of QMC sweeps while the change in $\text{Im} \Sigma(i\pi T)$ between iterations is controlled by the number of iterations. The iteration procedure is stopped when the change in $\text{Im} \Sigma(i\pi T)$ from iteration to iteration is less than the QMC statistical fluctuation of $\text{Im} \Sigma(i\pi T)$, $\delta_{\text{QMC}} \text{Im} \Sigma \simeq \delta \text{Im} G/(|\text{Im} G|)^2$. Notice that the QMC fluctuation of insulating solution is five to twenty times larger than QMC fluctuation of metallic solution as in Fig. 1 mostly because $\text{Im} G_{\text{ins}} \ll \text{Im} G_{\text{met}}$. This convergence criterion is more strict than the conventional one, which requires to stop iteration procedure when the norm of $||\text{Im} \Sigma^{(i+1)} - \text{Im} \Sigma^{(i)}||$ is smaller than a tolerance. For the conventional criterion underestimates the contribution of the most fluctuating component to the convergence by taking average of self energy differences between iterations over whole frequency range. The convergence criteria are illustrated in Fig. 1.

With this convergence criterion we performed the DMFT-QMC calculation to find solutions of a half-filled single-band Hubbard model at temperatures $T=1/57$, $1/64$, $1/100$, which turn out to be well below the critical temperature $T_c$. A careful selection of initial seeding to feed DMFT iteration is an essential part of finding the coexistence at finite temperature. At a given temperature, the best educated seeding is used to start DMFT iteration at initial value of interaction strength $U$: small interaction strength $U$ for metallic solution and large $U$ for insulating solution. After DMFT-QMC run we obtain convergent metallic and insulating solutions within a few iterations. We increase interaction strength $U$ by small increment (0.01) for metallic solution and decrease $U$ for insulating one. To reduce computational time, the convergent solution at the previous value of interaction strength $U$ is used as initial seeding for DMFT-QMC run at the next value of interaction strength $U$. We observe convergence pattern of solutions and repeat the procedures until critical slowing down is noticeably developed. By plotting inverse number of required iterations for the convergence of insulating solution in Fig. 2(a) and of metallic solution in Fig. 2(b), we identify upper bound of $U_{c1}(T)$ and lower bound of $U_{c2}(T)$. To find lower bound of $U_{c1}(T)$ and upper bound of $U_{c2}(T)$ we approach coexistence boundaries, $U_{c1}(T)$ and $U_{c2}(T)$, from outside the coexistence region. Outside the coexistence region only one solution exists. For interaction strength $U(T) < U_{c1}(T)$ DMFT iteration which starts with insulating seeding would produce convergent metallic solution. As $U$ gets closer to $U_{c1}$ from outside the coexistence region, convergence rate become slower. Such critical slowing down is clearly captured with open symbols in Fig. 2(a). By approaching coexistence boundaries from both inside and outside the coexistence region we obtain upper and lower bounds of $U_{c1}$ and $U_{c2}$ at several temperatures: for $\beta = 57$, $2.36 \leq U_{c1}(T) \leq 2.4$ and $2.42 \leq U_{c2}(T) \leq 2.53$; for $\beta = 64$, $2.36 \leq U_{c1}(T) \leq 2.41$ and $2.48 \leq U_{c2}(T) \leq 2.52$; for $\beta = 100$, $2.35 \leq U_{c1}(T) \leq 2.45$ and $2.58 \leq U_{c2}(T) \leq 2.62$.

At $\beta = 57$ the coexistence region is narrow enough so as to bring the critical slowing down into play over the whole coexistence region. Thus at temperatures above $\beta = 57$ the coexistence region could exist as well but will be inapproachable numerically for it is hard to achieve convergent solutions.

All known errors in DMFT-QMC should be reduced as much as possible in order to obtain irrefutable evidence of the coexistence. Those errors are the QMC statistical errors and the systematic errors. The latter originate from two sources: the finite sampling size errors in both direct $FT$ and $iFT$ and the Trotter finite size errors.

To reduce the finite sampling size errors in direct $FT$ we use cubic spline interpolation between grid points of Green’s functions. The main idea of cubic spline interp-
Correlation is to get an interpolating function that has continuous first and second derivatives at grid points. Boundary conditions are necessary to close the set of linear equations to determine interpolation function. The usual way, when boundary conditions are unknown, is to put the second derivatives at end points to zero (natural spline). In the system we treat we can obtain boundary conditions from Green’s function. To do so, we expand Green’s function \( G(\omega) \) via k-th derivatives of \( G(\tau) \) at end points: \[ G(\omega) = \sum_{k=0}^{\infty} (-1)^k (G^{(k)}(\tau^-) + G^{(k)}(\tau^+)) / (i\omega)^{k+1}. \]

One can also obtain correct high frequency behavior of Green’s functions using the moments of the spectral density \( \Pi \). Making correspondence between these two expansions we get the following formula for the second derivatives of Green’s functions in the case of half filled Hubbard model within DMFT: \( G^{(2)}(0^+) + G^{(2)}(\beta^-) = -(U^2/4 + t^2) \) for local Green’s function and \( G_{\nu}^{(2)}(0^+) + G_{\nu}^{(2)}(\beta^-) = -t^2 \) for Weiss function. The symmetry property of Green’s function at half filling is taken into account: \( G^{(k)}(0^+) = (-1)^k G^{(k)}(\beta^-) \).

Despite of a lot of frequency points used to define Green’s function \( G(\omega) \), the finite frequency cutoff in \( iFT \) results in removal of the discontinuity of \( G(\tau) \) at end points. To correct this situation we should extract \( 1/i\omega \) tail from Green’s function before making \( iFT \). To get correct \( iFT \) of \( G(\omega) \) one should make numerical \( iFT \) for \( G(i\omega - 1/i\omega) \) function and analytical \( iFT \) for the tail \( 1/i\omega \). In the case of half-filling the correct \( iFT \) is: \[ G(\tau) = T \sum_n e^{-i\omega_n \tau} [G(i\omega_n) - \frac{1}{i\omega_n}] - 1/2 \] for \( \tau > 0 \).

The corrections in direct \( FT \) and \( iFT \) are implemented in DMFT-QMC: correct boundary conditions in spline interpolation and tail correction in \( iFT \). All artificial oscillations at both \( \text{Im}\Sigma(\omega) \) and \( G(\tau) \) presented in DMFT-QMC without corrections disappears in DMFT-QMC with corrections.

Having implemented the corrections in DMFT-QMC, we perform DMFT-QMC run to get the coexistence at numerically most stable points, i.e., at mid-points between the coexistence boundaries. The statistical errors are reduced by increase of QMC sweeps per site up to \( 3 \times 10^5 \). Several DMFT-QMC calculations are performed with different values of \( \delta \tau (\approx \frac{1}{T}) \). Trotter errors are removed by extrapolation of data to the limit of \( \delta \tau \rightarrow 0 \). In Fig. 2 it is shown convergence of local Green’s function \( G(\tau) \) in the limit of \( \delta \tau \rightarrow 0 \). Insulating solutions are all within the QMC fluctuation \( (\sim 10^{-4}) \). However metallic solutions show monotonous increases with decreasing of \( \delta \tau \). In Fig. 3 it is shown convergence of double occupancy, \( \langle d \rangle = \langle n_x n_y \rangle \), as a function of \( \delta \tau^2 \). The convergence of metallic and insulating double occupancies in the limit of \( \delta \tau \rightarrow 0 \) confirms the coexistence within DMFT-QMC. In the limit of \( \delta \tau \rightarrow 0 \) we obtain \( \langle d_{\text{met}} \rangle \approx 0.039 \) and \( \langle d_{\text{ins}} \rangle \approx 0.026 \) for \( \beta = 64 \) and \( U = 2.44 \); \( \langle d_{\text{met}} \rangle \approx 0.036 \) and \( \langle d_{\text{ins}} \rangle \approx 0.023 \) for \( \beta = 100 \) and \( U = 2.53 \). With reducing all other finite size errors except ones originating from Trotter approximation, the effect of Trotter errors on the convergence of solution is found to be small compared to errors in direct \( FT \) and \( iFT \).

We now use our QMC results together with previous numerical results obtained with other methods to draw the phase diagram in Fig. 4. To supplement our QMC data, we use the estimates of the Mott endpoint within QMC \( \beta \). We also include estimates for the coexistence boundaries \( [3,2] \) from Exact Diagonalization(ED). At zero temperature, the value of \( U_{c2} \) was obtained with great accuracy in ref \( [3] \) using the projective self consistent method. Other exact methods such as the numerical renormalization group method(NRG) \( [7] \) give a very similar value for this quantity. The region near the Mott endpoint cannot be studied with numerically exact methods for the reasons discussed in this paper. However, we can use the Landau theory to scale the results of the IPT near the critical region as described in ref \( [8] \). This approach was used to determine the \( U_{c1}(T) \) and \( U_{c2}(T) \).
The physical meaning of the crossovers were discussed in ref. [15] in connection with experimental observations in $V$ ref. [15]. Two crossover lines above the Mott endpoint were scaled in a similar manner. The physical meaning of the crossovers were discussed in ref. [15] in connection with experimental observations in $V_2O_3$. Landau MIT line and crossover lines are mapped onto QMC phase diagram by shifting of $U_c$ and assuming an entropy difference of $ln(2)$ between the metallic and the insulating phase. The MIT lines obtained from those two methods agree well with MIT line obtained by ED method which we also included in Fig. 4. Given the systematic finite size errors of the various numerical approximations, it is clear that there is quantitative consensus (at the level of ten to twenty percent) between numerical calculations on where the coexistence region of fully frustrated Hubbard model in infinite dimensions lies. We note in passing, that the line of existence region of fully frustrated Hubbard model in infinite dimensions lies. We note in passing, that the line of existence region of fully frustrated Hubbard model in infinite dimensions lies. We note in passing, that the line of existence region of fully frustrated Hubbard model in infinite dimensions lies. We note in passing, that the line of existence region of fully frustrated Hubbard model in infinite dimensions lies. We note in passing, that the line of existence region of fully frustrated Hubbard model in infinite dimensions lies. We note in passing, that the line of existence region of fully frustrated Hubbard model in infinite dimensions lies. We note in passing, that the line of existence region of fully frustrated Hubbard model in infinite dimensions lies. We note in passing, that the line of existence region of fully frustrated Hubbard model in infinite dimensions lies. We note in passing, that the line of existence region of fully frustrated Hubbard model in infinite dimensions lies.

Near zero temperature, we determine the location of the finite temperature MIT line, by following ref. [13] and assuming an entropy difference of $ln(2)$ between the metallic and the insulating phase. The MIT lines obtained from those two methods agree well with MIT line obtained by ED method which we also included in Fig. 4. Given the systematic finite size errors of the various numerical approximations, it is clear that there is quantitative consensus (at the level of ten to twenty percent) between numerical calculations on where the coexistence region of fully frustrated Hubbard model in infinite dimensions lies. We note in passing, that the line of second order phase transitions reported in ref. [13] is actually crossover line at high temperature and the $U_{c2}(T)$ line at low temperature.

In conclusion, we find that QMC can be used to establish rigorously the existence of a coexistence region in the frustrated Hubbard model in infinite dimensions. Furthermore the numerical results are in full agreement with the predictions of the Landau theory of ref. [3] below $T_c$. Finally we notice that the methodology described in this paper should be useful when applying DMFT to other phase transitions in strongly correlated systems.

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