The Mott insulator – 10th order perturbation theory extended to infinite order using QMC

N. Blümel
Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany

E. Kalinowski
Department of Physics, Philips University, 35032 Marburg, Germany

(Dated: March 22, 2022)

We present a new method, based on the combination of analytical and numerical techniques within the framework of the dynamical mean-field theory (DMFT). Building upon numerically exact results obtained in an improved quantum Monte Carlo (QMC) scheme, 10th order strong-coupling perturbation theory for the Hubbard model on the Bethe lattice is extrapolated to infinite order. We obtain continuous estimates of energy $E$ and double occupancy $D$ with unprecedented precision $O(10^{-5})$ for the Mott insulator above its stability edge $U_{c1} \approx 4.78$ as well as critical exponents. The relevance for recent experiments on Cr-doped V$_2$O$_3$ is pointed out.

PACS numbers: 71.10.Fd, 71.27.+a, 71.30.+h

The exploration of the transition from a paramagnetic metallic phase to a paramagnetic Mott-Hubbard insulator is of fundamental interest in condensed matter theory. Essential features of this correlation phenomenon are captured by the single-band Hubbard model

$$
\hat{H} = - \sum_{\langle ij \rangle, \sigma} t_{ij} \left( \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma} \right) + U \hat{\mathcal{D}},
$$

(1)

where the operator $\hat{c}_{i\sigma}^\dagger$ ($\hat{c}_{i\sigma}$) creates (annihilates) an electron with spin $\sigma \in \{\downarrow, \uparrow\}$ on site $i$ and $\hat{\mathcal{D}} = \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$ counts the number of doubly occupied sites; $\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$. Its nonperturbative solution in the thermodynamic limit is possible within the framework of the dynamical mean-field theory (DMFT) which maps the lattice problem onto an Anderson impurity model; this mapping becomes exact in the limit of infinite dimensionality. The nature of the Mott-Hubbard transition in the idealized case of a fully frustrated Hubbard model with semi-elliptic noninteracting density of states (DOS) has been a matter of intense debate. As a result, a coexistence region of metallic and insulating solutions, enclosed by spinodal lines $U_{c1}(T) < U_{c2}(T)$, has been established below a critical temperature $T^* \approx 0.06t$. Only recently, estimates of energy $E = \langle \hat{H} \rangle/N$ and double occupancy $D = \langle \hat{\mathcal{D}} \rangle/N$ per lattice site have been obtained in quantum Monte Carlo (QMC) calculations with high enough precision for reliably pinpointing the first-order metal-insulator transition (MIT) line. A complete and universally accepted understanding of this prototype MIT is highly desirable (i) as a prerequisite for controlled studies of more material-specific aspects of such transitions (e.g., band structure, degree of frustration) and (ii) since already the single-band description can explain surprisingly many aspects of real-world experiments, which suggests a high degree of universality. In fact, recent experiments on V$_2$O$_3$ have not only found agreement with critical exponents at $T^*$ predicted by single-band DMFT, but even observed well-defined spinodal lines. The interesting question to what extent these lines can be identified with those computed in purely electronic models is still open; one criterion will be determined in this Letter.

In this work, we present results for the ground state insulating phase (“Mott insulator”) with unprecedented precision. After introducing the Kato-Takahashi strong coupling perturbation theory (PT) used for an exact calculation of all contributions to the energy including order $t^{10}/U^9$, we will sketch our advanced DMFT-QMC scheme which permits precisions of $O(10^{-5})$ (in $E/t$ or $D$) at selected phase points. The error bounds will be confirmed at moderately strong coupling ($U = 6t$). Finally, the breakdown of finite-order PT observed at smaller $U$ will be overcome using an extrapolation scheme to infinite order (“ePT”) which is controlled by its excellent agreement with QMC throughout the coexistence region. In addition to an estimate for $U_{c1}$ and to continuous estimates for $E$ and $D$ at all coupling strengths $U \geq U_{c1}$, we will extract critical exponents from ePT (which are clearly out of reach for both QMC and plain PT). Beyond the direct physical interest, our results will provide an essential reference in the (now very active) development of new methods for solving (multi-band) DMFT, its cluster extensions, and hybrid schemes such as LDA+DMFT. The infinite-order extrapolation method ePT constructed in this Letter is similar in spirit to Singh’s vastly successful extrapolation of $10^{th}$ order PT in $J_\perp/J_\parallel$ for the 2d Heisenberg antiferromagnet to the isotropic limit. The common general ideas appear promising for many areas of physics, potentially including QCD.

Perturbation theory – At half filling and in the absence of hopping, i.e. for $t_{ij} \equiv 0$ in , all states without double occupancies have the minimal energy $\langle U \hat{\mathcal{D}} \rangle = 0$; due to the arbitrariness of the spin direction on each site, the degeneracy of the space $\mathcal{D}_0$ of unperturbed ground states is $2^N$. An expansion around this strong-coupling limit
FIG. 1: Low order diagrams in PT: A first hopping process creates an empty site (circle). After a total of 2n hoppings, impacting n other sites (spheres), the ground state is restored.

at $T = 0$ using Kato’s formalism was established by Takahashi; for details in the case at hand, see Refs. 12 and 14. In this formalism, every ground state $\psi_n$ of $H$ is obtained by application of a well-defined operator $\Gamma$ on a state $\phi_n \in \mathcal{U}_0$: $\psi_n = \Gamma \phi_n$. Norm conservation implies $\Gamma^\dagger \Gamma = P_0$, where $P_0$ is the projector on $\mathcal{U}_0$. Thus, the Schrödinger equation $\hat{H} \psi_n = E_0 \psi_n$ may be written as

$$\hat{h} \phi_n = E_0 \phi_n, \quad \hat{h} \equiv \Gamma^\dagger \hat{H} \Gamma,$$

where $\hat{h}$ acts as an effective operator in the unperturbed space and can be expanded in orders of $t/U$:

$$\hat{h} = U \sum_{m=1}^{\infty} \hat{h}_m (t/U)^m.$$

The operators $\hat{h}_m$ generate electron transfers; since they have to preserve the absence of double occupancies, the associated diagrams are always closed. Specifically for the Bethe lattice, all closed paths are self-retracing. Neither unlinked diagrams nor diagrams of odd order in $t$ contribute (at half filling) for any lattice type [12]. Finally, graphs with more than two lines between any pair of sites are suppressed at least as $1/Z$. Fig. 1 illustrates the first three contributing orders. For the half-filled Hubbard model, the $m$th order Kato-Takahashi PT yields coefficients for a generalized Heisenberg model including up to $m$-site interactions. In the paramagnetic phase and for $Z = \infty$, an exact evaluation is possible since then all spin-spin correlation functions vanish. The 10th order result [13] obtained from a computer implementation of this diagrammatic approach will be discussed below.

Quantum Monte Carlo – Deep enough within the insulating phase, all excitations of the insulator are exponentially suppressed. Consequently, ground state properties can be estimated from measurements at finite (but small) temperatures $T$ (and vice versa); the precision can be tested and further increased in explicit extrapolations $T \to 0$. At finite $T$, the impurity part of the DMFT self-consistency problem may be solved using the auxiliary field quantum Monte Carlo (QMC) method; its accuracy is primarily limited by the discretization $\Delta \tau$ of the imaginary time $0 \leq \tau \leq T^{-1}$. In general, the $\Delta \tau$ error consists of the Trotter error and an error associated with discrete Fourier transformations (FT) performed twice per iteration of the DMFT self-consistency cycle. The FT error is essentially eliminated in a new high-precision QMC algorithm where the low-frequency physics of the impurity is obtained from QMC while the high-frequency part is computed analytically. This method converges much faster for $\Delta \tau \to 0$ at all frequencies than previously used methods [17]. The QMC results shown below are based on simulations at $T = 1/15$ for discretizations $0.09 \leq \Delta \tau \leq 0.25$ (with quartic extrapolation $\Delta \tau \to 0$) using some 40 iterations with $O(10^7)$ sweeps each. For $U \leq 5.0$, finite-$T$ corrections were estimated using additional simulations at $T = 1/20$ and $T = 1/25$ [18].

Results I – In the following, results are presented for the ground state (lower index 0 omitted). PT according to (2) and (3) (solid lines) in comparison with low-order PT (dashed/dotted lines) and QMC (circles).
Extended perturbation theory (ePT) – The idea of the ePT is an extrapolation of the coefficients \(a_n\) in the power series for the energy (for \(t = 1\)),

\[
E(U) = \sum_{i=1}^{\infty} a_{2i} U^{1-2i},
\]

from a small number of known coefficients \(a_2, \cdots, a_{n_0}\) to infinite order. Specializing on the case where all \(a_{2i}\) have the same sign \([21]\), we define the sequence

\[
U_{c1}[2i + 2] = \sqrt{a_{2i+2}/a_{2i}}. \tag{5}
\]

If this sequence converges, the ratio criterion implies the convergence of series \([4]\) for \(U > U_{c1} \equiv \lim_{n \to \infty} U_{c1}[2i]\) and divergence below. More specifically, we assume

\[
U_{c1}[n] = U_{c1} + u_1/n + u_2/n^2 + O(n^{-3}). \tag{6}
\]

Our assumption of this functional form will be strongly supported by fits to the known PT coefficients (cf. Fig. 3). By virtue of such a fit, series \([4]\) and its derivatives may be evaluated at arbitrary order. Comparisons of the numerical infinite-order limits of this scheme for \(E\) and \(D\) with QMC (cf. Fig. 4 and Fig. 5) will then give “numerical proofs” of the validity of \([21]\). Let us, however, first analyze the critical behavior: Eq. \((6)\) and \((5)\) imply \(a_n = a_{2i} U^{2i-n} = n^{-\tau}[c + O(1/n)]\), where \(\tau = -u_1/U_{c1}\). Re-expanding \([4]\) around the critical point \(U_{c1}\), we obtain

\[
E(U) = U_{c1} \sum_{i=1}^{\infty} a_{2i} (1 + x)^{1-2i}; \quad x \equiv \frac{U - U_{c1}}{U_{c1}},
\]

\[
= U_{c1} \left[ \left( \sum_{n=0}^{\infty} c_n x^n \right) + e_{1-\tau} x^{\tau-1} + e_{\tau} x^\tau + \ldots \right]. \tag{7}
\]

Note that any finite order in \([4]\) generates terms to all integer orders in \(x\) in \([7]\). The leading singular contribution to \(E\) is associated with \(e_{1-\tau} = \frac{\pi}{2\Gamma(1-\tau)}\). For the numerical step within the ePT we use weighted \([21]\) quadratic least squares fits to \([4]\) with either no adjustable parameters (“unrestricted” fit) or with minimal tuning of \(U_{c1}\) for enforcing analytic constraints or for obtaining error bounds from comparison with QMC. As seen in Fig. 3, the known coefficients (squares) are well represented by a “restricted” fit (solid line) to be discussed below. Its small curvature as well as slight deviations from the PT values become apparent only in the inset, where an average linear term has been subtracted. Also shown in the inset is the unrestricted fit (dashed line) which predicts \(U_{c1} = 4.75\) and \(\tau = 3.44\). The shaded region marks extrapolation curves which lead to estimates for \(E\) and \(D\) compatible with QMC; thus, QMC implies error bounds 4.72 \(\leq U_{c1} \leq 4.79\) and 3.36 \(\leq \tau \leq 3.53\). Half-integer exponents occur in the related Falicov-Kimball model \([22]\) and are generally expected in the context of mean-field theories. For our final estimates, we therefore assume an exponent \(\tau = 3.5\) in a restricted fit which implies \(U_{c1} = 4.782\) (in agreement with NRG \([22]\) and DMRG \([24]\) and corresponds to the solid lines in Fig. 3).

Results II – The ePT estimates for energy \(E\) and double occupancy \(D\) are shown in Fig. 4 and Fig. 5, respectively (solid lines); in the main panels, the 10th order PT results have been subtracted for enhanced clarity. These results agree perfectly with QMC (circles) which confirms the thermodynamic consistency of the latter \([19]\). In contrast, low order truncated ePT (dotted/dashed lines) deviates markedly, in particular for \(D\). The insets of Fig. 1 and Fig. 5 show contributions arising from the leading singular term in \([4]\) using \(e_{2.5} = -c_2 \sqrt[5]{\tau}\), where \(c \approx -0.00725\) is derived from the asymptotics of \(n^{3.5} a[n]\). These semi-analytic results agree well with the QMC/ePT estimates for contributions including and be-
beyond the leading critical term. Thus, the critical behavior is confirmed \textit{a posteriori} by QMC. The polynomial (in $x$) representation \cite{24} of the ePT results used in the above analysis is more accurate than $10^\text{th}$ order PT for $U < 6.6$ and should be used in future comparisons.\

\textit{Summary} – We have combined the strengths of high-order PT and of an improved QMC scheme and have constructed the ePT, an extension of PT to infinite order, in order to compute ground state properties of the Mott insulator within DMFT with unprecedented accuracy. We have confirmed earlier and independent estimates \cite{23,24} for the first time determined critical exponents ($5/4$ for $D - D_c$ and $3/4$ for $U$) \cite{24}

for $U_{c1}$, the lower (meta)stability edge of the insulator, and for the first time determined critical exponents ($5/2$ for $E$, $3/2$ for $D$). As both the spinodal line $U_{c1}(T)$ and the thermodynamic observables within the insulating phase are nearly $T$-independent (for $T \lesssim T^* / 2$), these results are also excellent approximations at finite temperatures where the MIT and both spinodal lines have been observed experimentally in Cr doped V$_2$O$_3$ \cite{4,5,8}. In particular, a comparison between experimental estimates for the critical exponents and our predictions could shed light on the still ill-understood role of the lattice at the transition. With the authoritative results for $E$ and $D$ provided by ePT and QMC \cite{27}, all details of the first-order Mott transition can now be clearly resolved which eliminates any room for alternative continuous-transition scenarios \cite{7}. Complementary results for the metallic ground state can be found in Ref. \cite{23} and various finite-temperature results will be published elsewhere.

We thank F. Gebhard for stimulating our interest in the subject, P.G.J. van Dongen for help in determining the critical exponents, and both as well as W. Ghuza, K. Held, E. Jeckelmann, and C. Knecht for discussions.

\begin{figure}[t]
\centering
\includegraphics[width=0.9	extwidth]{figure5.png}
\caption{Double occupancy from QMC (circles) and ePT (solid lines) in complete analogy with Fig. \ref{fig:fig3}.}
\end{figure}

\begin{thebibliography}{10}
\footnotesize
\item \bibitem{1} N. F. Mott, \textit{Metal-Insulator Transitions} (Taylor & Francis, 1990); F. Gebhard, \textit{The Mott Metal-Insulator Transition} (Springer, 1997); M. Imada, A. Fujimori, and Y. Tokura, Rev. Mod. Phys. \textbf{70}, 1039 (1998).
\item \bibitem{2} W. Metzner and D. Vollhardt, Phys. Rev. Lett. \textbf{62}, 324 (1989); A. Georges, G. Kotliar, W. Krauth, and M. Rozenberg, Rev. Mod. Phys. \textbf{68}, 13 (1996).
\item \bibitem{3} This DOS is realized on a Bethe lattice with nearest-neighbor hopping $t_1 = \sqrt{Z}$ for coordination $Z \to \infty$.
\item \bibitem{4} J. Schlifp, M. Jarrell, P. G. J. van Dongen, N. Blümer, S. Kehrein, T. Pruschke, and D. Vollhardt, Phys. Rev. Lett. \textbf{82}, 4890 (1999); M. J. Rozenberg, R. Chitra, and G. Kotliar, Phys. Rev. Lett. \textbf{83}, 3498 (1999); W. Krauth, Phys. Rev. B \textbf{62}, 6860 (2000); G. Kotliar, E. Lange, and M. J. Rozenberg, Phys. Rev. Lett. \textbf{84}, 5180 (2000).
\item \bibitem{5} R. M. Noack and F. Gebhard, Phys. Rev. Lett. \textbf{82}, 1915 (1999).
\item \bibitem{6} N. Blümer, Ph.D. thesis, Universität Augsburg (2002).
\item \bibitem{7} Claims based on RDA \cite[Ref. 20]{2}, FE-ED \cite{26}, and DMRG \cite{27} of a continuous MIT are clearly incompatible with this first-order scenario.
\item \bibitem{8} P. Limelette, A. Georges, D. Jerome, P. Wzietek, P. Metcalf, and J. M. Honig, Science \textbf{302}, 89 (2003).
\item \bibitem{9} G. Kotliar, Science \textbf{302}, 67 (2003).
\item \bibitem{10} R. R. P. Singh, Phys. Rev. B \textbf{39}, 9760 (1989).
\item \bibitem{11} T. Kato, Prog. Theor. Phys. \textbf{4}, 154 (1949).
\item \bibitem{12} M. Takahashi, J. Phys. C \textbf{10}, 1289 (1977).
\item \bibitem{13} M. P. Eastwood, F. Gebhard, E. Kalinowski, S. Nishimoto, and R. Noack, Eur. Phys. J. B \textbf{35}, 155 (2003).
\item \bibitem{14} E. Kalinowski, Ph.D. thesis, Universität Marburg (2002).
\item \bibitem{15} E. Kalinowski and W. Ghuza (2004), in preparation.
\item \bibitem{16} J. E. Hirsch and R. M. Fye, Phys. Rev. Lett. \textbf{56}, 2521 (1986).
\item \bibitem{17} C. Knecht, N. Blümer, and P. G. J. van Dongen (2004), in preparation.
\item \bibitem{18} Note that the insulating phase is thermodynamically stable at all phase points evaluated within QMC.
\item \bibitem{19} Note that within QMC $E$ and $D$ are essentially independent while $D = dE/dU$ within (e)PT by construction.
\item \bibitem{20} Oscillations observed in PT for finite $d$ would require, e.g., individual ePT fits for subsets of coefficients.
\item \bibitem{21} Fictitious errors $\Delta u_{c1}[n] \propto n^{-2}$ take the inaccuracy in $\Delta u_{c1}$ into account by overweighting higher-order PT data.
\item \bibitem{22} P. G. J. van Dongen, Phys. Rev. B \textbf{45}, 2267 (1992).
\item \bibitem{23} R. Bulla, T. A. Costi, and D. Vollhardt, Phys. Rev. B \textbf{64}, 045103 (2001).
\item \bibitem{24} D. J. Garcìa, K. Hallberg, and M. J. Rozenberg, Preprint cond-mat/0403169 (2004).
\item \bibitem{25} Further support for half-integer exponents comes from the next term in \cite{29} which we (EK) calculated after submission as 4496245/2048714; its inclusion in an unrestricted fit increases the numerical estimate to $\tau = 3.46$.
\item \bibitem{26} The coefficients in \cite{29} are in terms of $\tilde{c}_n \equiv U_{c1} c_n$ (for $U_{c1} = 4.782$): $\tilde{c}_0 = -0.1107586$, $\tilde{c}_1 = 0.1302062$, $\tilde{c}_2 = -0.2213925$, $\tilde{c}_{2.5} = 0.18536$, $\tilde{c}_3 = 0.04532$, $\tilde{c}_{3.5} = -0.13$, $\tilde{c}_4 = 0.03406$, $\tilde{c}_5 = 0.03759$, $\tilde{c}_6 = -0.03$.
\item \bibitem{27} Very recently, our ePT results for $E$ have been reproduced at $U = 4.8, 5.6$ within $O(10^{-6})$ using SFT/DIA \cite{28} [Požgačič, cond-mat/0407172; private communication].
\item \bibitem{28} N. Blümer and E. Kalinowski (2004), to appear in Physica B; preprint cond-mat/0407442.
\end{thebibliography}

* Electronic address: Nils.Bluemer@uni-mainz.de