An effective classical correspondence of the Mott transition

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We derive an effective classical model to describe the Mott transition of half-filled one-band Hubbard model in the framework of the dynamical mean-field theory with hybridization expansion of the continuous time quantum Monte Carlo. We find a simple two-body interaction of exponential form and reveal a classical correspondence of the Mott transition driven by a logarithmically divergent interaction length. Our work provides an alternative angle to view the Mott physics and suggests a renewed possibility to extend the application of the quantum-to-classical mapping in understanding condensed matter physics.

Mott transition is arguably one of the most fundamental concepts of correlated electrons and has been extensively investigated during the past decades [1–12]. In the framework of the dynamical mean-field theory (DMFT), it was predicted to be a first order transition with a coexisting insulating and metallic regime below the critical end point [13–16]. This has been confirmed experimentally in transition metal oxides such as V$_{2-x}$Ti$_x$O$_3$ [17], in which a systematic analysis of the conductivity has revealed a scaling behavior near the critical end point resembling that of the liquid-gas transition [18]. It is therefore natural to ask if and how the Mott system can be mapped to a classical liquid-gas system.

The quantum-to-classical mapping has made important contributions in the history of condensed matter physics [19–34]. The mapping is a generic property of quantum statistical mechanics, but often limited by complex series expansion of the partition function. We show that such a situation may be improved with the help of lately-developed machine learning approach. The latter has led to rapid progresses [35] in identifying phase transitions, speeding up quantum Monte Carlo simulations [36–42], constructing many-body ground states [43–46], and optimizing tensor networks [51–53]. In this work, we explore the possibility of using the machine learning technique to construct a classical correspondence of the Mott system within the DMFT framework. We find that the quantum model can be mapped to a classical molecular gas with an effective two-body potential of an exponential form. The Mott transition is then in correspondence with the classical liquid-gas transition tuned by the range of the inter-molecular interaction.

For simplicity, we discuss the Mott transition based on the one-band Hubbard model at half filling,

$$H = -t \sum_{\langle ij \rangle, \sigma} \left( c_{i \sigma}^\dagger c_{j \sigma} + \text{H.c.} \right) + U \sum_i (n_{i \uparrow} - \frac{1}{2})(n_{i \downarrow} - \frac{1}{2}),$$

where $t$ is the hopping integral and $U$ is the onsite Coulomb interaction. In the framework of DMFT, the lattice problem is mapped to an impurity problem coupled with a self-consistent bath. We then solve the impurity model using the continuous time quantum Monte Carlo method with hybridization expansion (CT-HYB) [54, 55]. The partition function of the impurity model has the form,

$$Z \propto \sum_{k, k=0}^{\infty} \int_0^\beta \prod_{i=1}^k (d\tau_i d\tau'_i) \prod_{j=1}^k (d\tilde{\tau}_j d\tilde{\tau}'_j) \omega_{\text{loc}} \omega_{\text{hyb}},$$

where $\omega_{\text{loc}} = e^{U(L_{\text{tot}}/2 - \text{O}_{\text{tot}})}$ and $\omega_{\text{hyb}} = |\text{det} M^{-1}(\Delta)|$ are the local and hybridization weights for the configuration, $\{C_k : \tau_1, \tau'_1 \ldots ; \tau_k, \tau'_k\}$ and $\{C_k : \tilde{\tau}_1, \tilde{\tau}'_1 \ldots ; \tilde{\tau}_k, \tilde{\tau}'_k\}$ of the two spin channels. $k$ and $\tilde{k}$ are their orders of expansion, respectively. In CT-HYB, as shown in Fig. 1 $L_{\text{tot}}$ is the sum of the lengths of all segments (solid line) and $O_{\text{tot}}$ accounts for the overlap (shaded area) between

![FIG. 1: Mapping between the CT-HYB configuration and the classical configuration of charged particles. For CT-HYB, the full and empty circles at the imaginary times $\tau_i$ ($\tilde{\tau}_i$) represent the creation and annihilation operators of spin up (down), respectively. The shaded areas indicate the overlap between the segments (solid lines) of two spin channels. In the classical model, the circles represent charged particles on a unit circle at $x_i^+ = \tau_i/\beta$, $x_i^- = \tau_i'/\beta$, $\tilde{x}_i^+ = \tilde{\tau}_i/\beta$ and $\tilde{x}_i^- = \tilde{\tau}_i'/\beta.$](image-url)
segments of different spins. $M^{-1}(\Delta)$ is a $(k+\bar{k}) \times (k+\bar{k})$ matrix of the hybridization function $\Delta$ in imaginary time. Absent spin flip, the two spin channels are separated such as $\omega_{\text{hyb}} = \omega^\sigma_{\text{hyb}}(C_k)\omega^\bar{\sigma}_{\text{hyb}}(\bar{C}_k)$. We have chosen CT-HYB rather than the interaction expansion (CT-INT) as the impurity solver for two reasons [48]. In CT-INT, each configuration $\{C_k : \tau_1, \ldots, \tau_k\}$ corresponds to a collection of interaction vertices, whose Boltzmann weight, $\omega(C_k) \propto (-U)^k$, is only positive for all $k$ for $U < 0$ and therefore improper for studying the Mott transition. Secondly, CT-INT has only one type of particles and requires three-body interactions to prevent collapse of classical simulations, while CT-HYB contains both creation and annihilation operators, which may be regarded as charged particles in the classical model and allow us to consider only the two-body interaction.

We first focus on the hybridization part, $\omega_{\text{hyb}}$. The local part, $\omega_{\text{loc}}$, has already a classical form. Because of the spin symmetry, the two spin channels follow the same probability distribution function. We will only discuss one spin channel and later consider their combination through $\omega_{\text{loc}}$. As shown in Fig. [1](a), each spin channel is mapped onto a circle. If we regard the creation (annihilation) operators at the imaginary time $\tau_i$ ($\tau^\prime_j$) as a positive (negative) charge $q_i = (+)$ (-), the CT-HYB configurations are mapped to an ensemble of charged particles. The question is if a classical model may be constructed to reproduce the quantum weight of each configuration. For this, we first make the simplest assumption of two-body interactions and propose an energy function,

$$E_{\text{eff}}(C_k) = -\frac{1}{2} \sum_{i,j; l,j,q} V_{q,j}(x_{ij}^q - x_{ij}^{q'}) + \mu_{\text{eff}}k + E_0, \quad (3)$$

where $V_{q,j}(x_{ij}^q - x_{ij}^{q'})$ is the two-body potential depending on the charges and distance of two different classical particles, $E_0$ is a constant background energy, and $\mu_{\text{eff}}$ is an effective chemical potential of the classical model coupled to the number $k$ of charged pairs, which should not be confused with the usual chemical potential of the Hubbard model. $\sum'$ indicates that the self-interaction is excluded in the sum. To determine the exact form of the potential function, we use the Legendre expansion, $V_{q,j}(x) = \sum_{l=0} P_l(2x - 1)$, where $0 \leq x \leq 1$ and $P_l(x)$ is the $l$-th order Legendre polynomial. The classical model is then fully determined by the parameters $V_{q,j}$ (up to a sufficiently large cutoff of $l$) and $\mu_{\text{eff}}$, which can be trained with linear regression by requiring $-E_{\text{eff}}(C_k)$ to match $\ln\omega_{\text{hyb}}(C_k)$ for all tested CT-HYB configurations.

We have collected 250,000 samples for each set of parameters, computed their log-weights as the regressing target, and then applied ridge regression with $L_2$ regularization of the strength $10^{-3}$ to prevent overfitting.

Figure [2](a) gives the typical results for the Bethe lattice with a half bandwidth $D = 2$, the Coulomb interaction $U = 3$, and the inverse temperature $\beta = 30$. As shown in Figs. [2](a) and [2](b), we obtain an excellent agreement between the effective energy function and the calculated log-weight. The proposed classical model indeed captures the quantum distribution of the original Hubbard Hamiltonian. The Legendre coefficients $V_{q,j}$ are plotted in Fig. [2](c). The rapid decay of their magnitude for large $l$ confirms the validity of the expansion. Figure [2](d) compares the derived two-body interactions, $V_{q,j}(x)$, as functions of distance. The plot reveals a number of interesting symmetries in $V_{q,j}$, which may be rationalized as follows. First, for a classical model, one typically expects $V_{q,j}(x) = V_{q,j}(x) = V_{q,j}(1 - x)$ between any two particles on the unit circle. Second, inserting a segment whose length approaches zero should not change the total energy. In the quantum Monte Carlo simulations, this operation does not generate a new configuration and is therefore typically not considered. However, in the classical model, this corresponds to the situation of adding a pair of particles of opposite charges at the same location, whose interactions with any third particle should always cancel. The latter implies a generic rule of the classical interactions between charged particles, namely, $V_{++} = V_{--} = -V_{+-} = -V_{-+} = -q_i q_j V(x)$. Third, it immediately follows from the above constraints that the interaction $V(x)$ must be symmetric with respect to $x = 1/2$, namely, $V(x) = V(1 - x)$ for $0 \leq x \leq 1$.

The functional form of $V(x)$ thus provides key information on the classical particle system. Quite unexpectedly, as shown in Fig. [3](a), we find that it can be well fitted...
with an exponential function for all parameter regimes of $U$ and $\beta$ regardless of the metallic or insulating phases:

$$V(x) = V_0 e^{-\min(x,1-x)/\xi} + V_1,$$

where $V_0$ and $V_1$ are both constants and $\xi$ reflects an effective range of the two-body interaction. This suggests that the simple form captures the essential physics of the hybridization function. Since we are dealing with the self-consistent bath coupled to the impurity, the exponential decay seems to imply that the lattice effect is to screen the local correlation on a finite length (or imaginary time) scale $\xi$. It will be interesting to see if such a form may still be valid in more general cases such as away from half filling or with multiple orbitals. Our analyses seem independent of these details as long as the model does not contain any spin or orbital mixing.

The above potential can be further simplified by removing the constant term $V_1$. Since the charged particles always appear pairwise in CT-HYB configurations, the overall effect of $V_1$ on the total energy is nothing but a term, $-V_1 k$, which can be absorbed by redefining $(\mu_{\text{eff}} - V_1) \rightarrow \mu_{\text{eff}}$ in Eq. (3). Moreover, imagining that we insert again $N$ segments of almost zero length, the variation of the total energy should also be zero, namely $\delta E_{\text{eff}} = -V_0 N + \mu_{\text{eff}} N = 0$. This requires $\mu_{\text{eff}} = V_0$, which was first found unexpectedly in all our fittings.

We have thus only two parameters in the effective model and the total energy function adopts a very simple approximate form,

$$E_{\text{eff}}(\mathcal{C}_k) - E_0 = \frac{V_0}{2} \sum_{i,q;i,j,q_j} q_i q_j e^{-\delta q_j q_i / \xi},$$

where the $k$-term is absorbed as a self-interaction for $i = j$ and $q_i = q_j$ and the distance between two charged particles is defined as, $\delta q_i q_j = \min(|x_{ij}^q - x_{ij}^q|, 1 - |x_{ij}^q - x_{ij}^q|)$, including self-interaction. This energy function incorporates faithfully the major effect of the lattice correlations on the local impurity model in the DMFT iterations. For examination, we have inserted it back into the Monte Carlo simulations after the parameters were determined with a small set of training samples, the results agree well with the pure quantum simulations.

Thus all informations on the Mott transition are squeezed into the interaction potential, $V_0$, and its effective range, $\xi$, in the classical model. To study how these two parameters behave across the Mott transition, we plot in Fig. 4(b) their variations as a function of $U$ for $\beta =$10, 20, 50, which are above, near and below the Mott critical end point, respectively. The results were obtained by gradually increasing $U$ from $U = 0$ in the metallic side to $U = 8$ in the insulating side and then annealing back to the metallic state. For each $U$, we took the input from the converged solution of previous $U$ at the same $\beta$. As expected, we see a jump and a clear hysteresis at $\beta = 50$. 

FIG. 3: (a) Exponential fit of the effective potential for different values of $U$ and $\beta$, showing excellent agreement in all three regimes. (b) The fitting values of $V_0$ and $\xi$ in the classical model after DMFT convergence with gradually increasing (> ) or decreasing (< ) $U$.

FIG. 4: (a) Variations of $V_0$ as functions of $\beta$ and $U$, showing a rapid change across the Mott transition and slight change in other parameter regime. The arrows indicate the direction of decreasing (solid line) or increasing (dashed line) $U$ for the DMFT calculations. The dotted lines mark the region of numerical hysteresis of the first-order transition. (b) The pair number, $\langle k \rangle$, as a function of the inverse temperature $\beta$ for different values of $U$, showing the change of the pair density, $d\langle k \rangle / d\beta$, across the Mott transition.
in both parameters due to the first-order nature of the Mott transition. For \( \beta = 10 \) above the Mott critical end point, the jump turns into a smooth crossover and both parameters vary continuously with \( U \).

The overall variation of \( V_0 \) with respect to the original parameters \( U \) and \( \beta \) is summarized in Fig. 3(a). Surprisingly, we see \( V_0 \) only undergoes a rapid change of roughly the factor of 3 across the transition and otherwise varies only slightly with \( U \) and \( \beta \). This is reminiscent of the volume change in the classical liquid-gas transition. \( V_0 \) thus plays a passive role in the phase transition of the classical model. Interestingly, as shown in Fig. 3(b), the particle number \( \langle k \rangle \) as a function of \( \beta \) changes its slope across the transition such that the particle density \( \rho = d\langle k \rangle/d\beta \) also jumps from roughly 0.3 in the metallic state and 0.1 in the insulating state, just the opposite of that of \( V_0 \).

It is therefore speculated that \( \xi \) is the primary driving force for the phase transition. Figure 3(a) plots the parameter flow in the \( V_0 - \xi \) space for both increasing and decreasing \( U \) at \( \beta = 50 \). While \( V_0 \) changes only slightly in each phase, we see \( \xi \) varies greatly until a sudden transition is triggered. Since \( \xi \) represents the effective range of the two-body interaction, the transition is therefore controlled by the scattering length between two charged particles. As a matter of fact, as shown in Fig. 3(b), we find a logarithmic dependence, \( \xi \sim \pm \ln |1 - U/U_c| \) from either side of the phase diagram. This indicates that the effective interaction becomes progressively short or long range approaching the Mott transition. From the metallic side, the potential turns gradually local as \( U \rightarrow U_{c1} \) and the particles become asymptotically free before they expand into the gas state; while starting from the insulating side, \( \xi \) becomes gradually divergent as \( U \rightarrow U_{c2} \) and the particles get more and more correlated until they eventually condense into a liquid. Thus the Mott metal-to-insulator transition corresponds roughly to a classical liquid-to-gas transition controlled by the single parameter \( \xi \).

The classical correspondence provides to some extent an alternative angle to view the spin and charge dynamics of the Mott physics. One should combine the two spin channels through the local weight \( \omega_{loc} \) into a single circle. Since \( U \) is large, all the segments are intended to cover together the whole circle to reduce the Coulomb energy. Thus each charged particle is roughly bound to a nearby particle of opposite spin and charge. Then the CT-HYB configurations are reduced to a single circle and the corresponding classical model turns into a gas of diatomic molecules with an additional intra-molecular potential \( V_m(x) \propto \sum_{i,q} [x_{r_i}^{q_i} - x_{c_i}^{q_i}] \). The charge and spin fluctuations correspond to the internal and global configurations of the molecular gas, respectively. We should note that despite the good agreement of the energy function, the classical model should by no means be viewed as an exact representation of the quantum model. It might not be able to reproduce certain subtle properties of the original model, in particular the long-time dynamics in the very vicinity of the critical end point. Nevertheless, its simple and explicit form may still capture some truth of the underlying physics. For numerical studies, our energy function may be applied as a reference system for the quantum simulations. As discussed in Ref. [48], once the parameters are obtained with a relatively small number of test configurations, the Monte Carlo simulations may be accelerated by an improved acceptance probability \( p(C \rightarrow C') = \min \left\{ 1, \frac{e^{-U_{eff}(C')/\beta} \omega(C')}{e^{-U_{eff}(C)/\beta} \omega(C)} \right\} \).

To summarize, we have constructed an effective classical correspondence for understanding the Mott transition of the half-filled Hubbard model in the framework of DMFT with the CT-HYB algorithm. The derived model may be regarded as a charged molecular gas with a simple two-body interaction of the exponential form. Our analysis suggests that the Mott transition may correspond to a classical liquid-gas transition of the molecules driven by the effective range of the particle interaction. The correlation length exhibits logarithmic behaviors approaching the transition. It should be noted that the above picture was derived in the framework of DMFT. For an exact lattice treatment, the quantum model in \( d \) spatial dimension corresponds to a classical model in \( d+1 \) dimension. Then one may ask if similar two-body interactions will still be valid, possibly with anisotropic correlation lengths, \( \xi_{eff} \), whose values reflect the screening of the Coulomb potential.
tial along different spatial or temporal axes. A verification of this scenario demands numerical simulations of the lattice model using more sophisticated approaches.

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