Slave rotor theory of the Mott transition in the Hubbard model: a new mean field theory and a new variational wave function

Tao Li$^1$, Tomonori Shirakawa$^{2,4}$, Kazuhiro Seki$^{2,3}$ and Seiji Yunoki$^{2,3,4}$

$^1$Department of Physics, Renmin University of China, Beijing 100872, P.R.China
$^2$Computational Condensed Matter Physics Laboratory, RIKEN, Wako, Saitama 351-0198, Japan
$^3$Computational Materials Science Research Team, RIKEN Advanced Institute for Computational Science (AICS), Kobe Hyogo 650-0047, Japan
$^4$Computational Quantum Matter Research Team, RIKEN Center for Emergent Matter Science (CEMS), Wako, Saitama 351-0198, Japan

(Dated: January 12, 2016)

A new mean field theory is proposed for the Mott transition in the Hubbard model based on the slave rotor representation of the electron operator. This theory provides a better description of the role of the long range charge correlation in the Mott insulating state and offers a good estimation of the critical correlation strength for the Mott transition. We have constructed a new variational wave function for the Mott insulating state based on this new slave rotor mean field theory. We find this new variational wave function outperforms the conventional Jastrow type wave function with long range charge correlator in the Mott insulating state. It predicts a continuous Mott transition with non-divergent quasiparticle mass at the transition point. We also show that the commonly used on-site mean field decoupling for the slave rotor corresponds to the Gutzwiller approximation for the Gutzwiller projected wave function with only on-site charge correlator, which can not describe the Mott transition in any finite dimensional system.

PACS numbers:

The study of Mott transition and the possible quantum spin liquid ground state around the Mott transition point in Hubbard type models has attracted a lot of attention in the strongly correlated electron system community. The organic compound with the formula $\kappa-(ET)_2Cu_2(CN)_3$ forming a triangular lattice is particularly interesting in this respect. It is generally believed that the multi-spin exchange process in the intermediate correlation regime may be crucial for the stabilization of the quantum spin liquid ground state. Measurements on $\kappa-(ET)_2Cu_2(CN)_3$ seem to support such an expectation. More recently, the possibility of quantum spin liquid ground state around the Mott transition has also been hotly discussed for Hubbard models with a Dirac-type electron dispersion.

The study of the spin liquid state in Hubbard models is more complicated than in Heisenberg models as a result of the added complexity of the charge degree of freedom. Depending on the value of $U$ for charge gap opening, the Hubbard model can exhibit different physics in the intermediate coupling regime. The spin liquid phase is possible only when the charge gap opens before other symmetry breaking transition. Thus, an accurate estimation of the Mott transition point is important in the study of spin liquid phase in Hubbard models. The Jastrow-type variational wave function is a commonly used way to describe such a non-symmetry breaking transition. The Jastrow wave function is composed of the product of the Slater determinant $|\Psi_{FS}\rangle$ for the free electron and a Jastrow factor describing the charge correlation in the system. Previous studies find that to describe the Mott transition from the metallic phase, the Jastrow factor must be long ranged. In particular, the long range charge correlation is responsible for the binding of the holon(empty site) and the doublon(doubly occupied site) in the Mott insulating state. While physically appealing, there is no microscopic justification for the use of the heuristic form of the Jastrow factor, except in one dimension, when the collective charge fluctuation is the only important correction at low energy beyond the free fermion ground state. At the same time, a very large system is needed to see clearly the signature of Mott transition in the Jastrow wave function, which is governed by the long wavelength physics.

The slave rotor representation of the electron operator is an economic way to describe the charge degree of freedom of the Hubbard model and is widely used in the study of the Mott transition of the Hubbard systems. Different estimations on the critical value $U_c$ of the Mott transition have been made using various kind of mean field treatment of the slave rotor. In the simplest on-site mean field approximation, the Mott transition is approached when both the coherent weight and the band width of the quasiparticle excitation vanish. This is believed to be true only in the limit of infinite dimensions, when the spatial correlation is irrelevant. This problem can be solved by a large-N treatment of the U(1) charge rotor, in which the unitary constraint on the charge rotor is relaxed to a requirement on the average. However, it is not clear to what extent the approximations adopted on the rotor are relevant for electron in the original Hubbard model, since the mean field theory breaks the U(1) gauge symmetry inherent in the slave rotor representation. Especially, it is not clear what is the relation between the various mean field theories with the variational approaches.

The purpose of this paper is to bridge the variational approach and the slave rotor theory. In this paper, we...
propose a new mean field theory for the Hubbard model in the slave rotor representation. The new mean field treats better the long range charge correlation and predicts a continuous Mott transition for Hubbard model with non-divergent quasiparticle mass at the transition point. We then construct explicitly the variational wave function related to this slave rotor mean field theory by enforcing the rotor constraint on the slave rotor mean field ground state. The so constructed wave function can be written as the product of a permanent for the charge sector and a Slater determinant for the spin sector. We have performed variational Monte Carlo simulation on this new wave function and find that it outperforms the Jastrow wave function with long range correlator in the Mott insulating state, although it involves two variational parameters. At the same time, we find that the widely used on-site mean field approximation for the slave rotor generates the simple Gutzwiller wave function of the form \( g^D |\Psi_{FS}\rangle \), which is not suitable for the description of Mott transition in finite dimensional systems.

In the slave rotor representation, the electron operator is written as

\[
c_i,\sigma = e^{-i\theta} f_i,\sigma. \tag{1}
\]

Here \( e^{-i\theta} \) is the lowering operator of a U(1) rotor that describes the charge degree of freedom of the electron, and \( f_i,\sigma \) is the fermionic spinon operator that describes the spin degree of freedom of the electron. To recover the correct Hilbert space and the algebra among \( c_i,\sigma \) and \( c_i^\dagger,\sigma \), the rotor and the spin degree of freedom should be subjected to the following constraint

\[
L_i = \sum_\sigma f_i^\dagger,\sigma f_i,\sigma - 1. \tag{2}
\]

Here \( L_i \) is the angular momentum of the slave rotor on site \( i \) and is conjugate to phase variable \( \theta_i \).

We consider the Mott transition of the Hubbard model of the form

\[
H = -t \sum_{<i,j>,\sigma} c_i^\dagger,\sigma c_j,\sigma + U \sum_i n_i,\uparrow n_i,\downarrow, \tag{3}
\]

here \( n_i,\uparrow = c_i^\dagger,\uparrow c_i,\uparrow \), \( n_i,\downarrow = c_i^\dagger,\downarrow c_i,\downarrow \). In the slave rotor representation, up to a constant and a shift in chemical potential, the model can be written as

\[
H = -t \sum_{<i,j>,\sigma} f_i^\dagger,\sigma f_j,\sigma e^{i(\theta_i - \theta_j)} + U/2 \sum_i L_i^2. \tag{4}
\]

Here we have exploited the rotor constraint to rewrite the interaction term as the kinetic energy of the slave rotors. The form of the Hamiltonian is inviting to decouple the spinon degree of freedom and the rotor degree of freedom. This results in the following effective Hamiltonian for the rotor and the spinon

\[
H_s = -t_f \sum_{<i,j>,\sigma} f_i^\dagger,\sigma f_j,\sigma \tag{5}
\]

and

\[
H_r = -J \sum_{<i,j>,\sigma} e^{i(\theta_i - \theta_j)} + U/2 \sum_i L_i^2, \tag{6}
\]

respectively, where \( t_f = t < e^{i(\theta_i - \theta_j)} > \) and \( J = J < \sum_\sigma f_i^\dagger,\sigma f_j,\sigma > \). After such a decoupling, the spinon part becomes a free fermion systems and has the same Hamiltonian as the free electron. It can then be shown that at the zero temperature \( J = \frac{Z}{N} \), in which \( K \) is the absolute value of the ground state energy of the non-interacting system on the same lattice, \( Z \) and \( N \) are the coordinate number and the total number of sites of the lattice respectively.

The rotor part is still nontrivial and further approximation is needed to solve it. In the commonly used on-site mean field approximation, one takes \( x = < e^{i\theta} > \) as a site-independent constant. The decoupled rotor Hamiltonian then becomes the sum of independent rotors

\[
H_\theta = -K x \sum_i \cos \theta_i + U/2 \sum_i L_i^2. \tag{7}
\]

This model can exhibit two phases depending on the value of \( \frac{U}{K} \). In the small \( U \) limit, the rotor will break the U(1) rotational symmetry and \( x \) will be nonzero. This corresponds to a metallic phase in which both the spinon band width and the quasiparticle weight are renormalized by a factor \( x \). On the other hand, when \( U \) is large enough, the rotor will recover the U(1) rotational symmetry and \( x \) will become zero. In such a case, both the spinon band width and the quasiparticle weight will be zero. The critical value \( U_c \) for such a transition can be obtained from the self-consistent equation \( x = < e^{i\theta} > \) and is given by \( U = 2K \). On the triangular lattice this corresponds to \( U_c \approx 4.7t \).

The on-site mean field treatment can provide a rough understanding of the Mott transition on the triangular lattice. However, the critical value \( U_c \) for the Mott transition predicted by it is much smaller than that is generally expected. The divergence of the spinon effective mass at the Mott transition is also not generally accepted for a finite dimensional system. Another way to see the insufficiency of the on-site mean field approximation is to study the related variational wave function, which can be constructed by enforcing the rotor constraint on the mean field ground state. The mean field wave function of the system in the rotor representation is given by

\[
|MF> = \prod_i \left( \sum_{m_i} \phi_{m_i} |m_i> \right) |f - FS> , \tag{8}
\]

in which \( |f - FS> \) denotes the spinon Fermi sea, \( \phi_{m_i} \) is the rotor wave function on site \( i \). The true wave function of the system is given by \( |\Psi> = \prod_i P_i |MF> \), in which \( P_i \) is the projector enforcing the rotor constraint Eq.(2) on site \( i \). Since the spinon occupation number on a given site can only be 1 or 2, the rotor angular momentum
m_i can only be 0, 1 or -1. In such a case, |Ψ⟩ reduces to the usual Gutzwiller projected wave function of the form \( g^D |Ψ_{FS}⟩ \), with the factor \( g \) given by \( g = φ_{±1}/φ_0 \).

Here \( D \) is number of doubly occupied sites in the system. As is well known, the simple Gutzwiller projected wave function can not describe the Mott transition in any finite dimension. Only in the limit of infinite dimensions, when the Gutzwiller projector can be treated exactly with the Gutzwiller approximation, the Gutzwiller wave function can predict a Mott transition at finite \( U \). At the same time, the divergence of spinon effective mass is realized only in the limit of infinite dimensions, when all spatial correlation can be neglected. We thus conclude the on-site slave rotor mean field approximation is equivalent to the commonly used Gutzwiller approximation and can not describe the Mott transition in finite dimensions.

The reason for the failure of the simple Gutzwiller wave function to describe the Mott transition in finite dimension is that the long range charge correlation, which has been proved to be crucial for a correct theory of Mott transition, is not properly accounted for in such a local treatment. The main effect of such long range charge correlation is to introduce attraction between the holon(empty site) and the doublon(doubly occupied site) in the singly occupied background. In the Mott insulating state, the holon and doublon will be bounded together because of such attraction. For smaller \( U \), the holon-doublon pair will disassociate and the system will become metallic. To restore such long range charge correlation in the variational wave function, various kinds of charge correlator have been proposed. In particular, the long range Jastrow factor has been extensively adopted in the study of the Mott transition in Hubbard models. However, the Jastrow factor is constructed from a two-body consideration and is heuristic in nature. In the following, we propose a new charge correlator based on a new type of slave rotor mean field theory. The new mean field theory overcomes the drawbacks of the on-site rotor mean field theory and predicts a non-divergent effective mass at the Mott transition. The \( U_c \) predicted by the new theory is also more reasonable.

To formulate the new mean field theory, we introduce a boson representation of the rotor degree of freedom. As a result of the rotor constraint, the angular momentum of the rotor can only be 0 or ±1. Here we introduce three boson operators \( b_0 \) and \( b_{±1} \) to represent these three states. The three bosons are thus subjected to the constraint of

\[
\sum_\alpha b_\alpha^\dagger b_\alpha = 1, \tag{9}
\]

in which \( \alpha = 0, ±1 \). We note that the three bosons carry different charges. More specifically, \( b_{i,\alpha} \) carries charge \( \alpha \) relative to the singly occupied background. With these boson operators, the rotor Hamiltonian can be written as

\[
H_r = -J \sum_{<i,j>} (s_i^+ s_j^- + s_i^- s_j^+) + \frac{U}{2} \sum_i (n_i,1 + n_{i,-1}), \tag{10}
\]

in which \( n_{i,\alpha} = b_{i,\alpha}^\dagger b_{i,\alpha}, \quad s_i^+ = b_{i,1}^\dagger b_{i,0} + b_{i,0}^\dagger b_{i,-1}, \quad s_i^- = b_{i,1}^\dagger b_{i,0} + b_{i,0}^\dagger b_{i,1}. \)

In the large \( U \) limit, most sites will be singly occupied and we expect both \( n_{-1} \) and \( n_1 \) to be small. We thus assume \( b_0 \) condenses and treat it as a c-number to be determined self-consistently from the constraint. The rotor Hamiltonian then becomes

\[
H_r = -J \eta \sum_{<i,j>} (b_{i,1}^+ b_{j,1} + b_{i,-1}^+ b_{j,-1} + h.c.) + U \sum_i (n_{i,1} + n_{i,-1}). \tag{11}
\]

in which \( \eta = |⟨b_0⟩|^2 \). Here we note that the condensation of \( b_0 \) does not break the U(1) rotational symmetry of the rotor since it carries zero charge.

The above Hamiltonian can be diagonalized to give

\[
H_r = \sum_k \epsilon_k (\beta_{k,1}^+ \beta_{k,1} + \beta_{k,-1}^+ \beta_{k,-1}) + \text{const.} \tag{12}
\]

Here \( \epsilon_k = \sqrt{\xi_k^2 - \Delta_k^2} \), in which \( \xi_k = \frac{U}{2} - JZ \gamma_k \) and \( \Delta_k = JZ \gamma_k \). \( \gamma_k = \frac{1}{2} \sum_i e^{ik·}\xi_i, \) where \( \xi_i \) denotes the vectors connecting nearest neighboring sites on the lattice. The value of \( \eta \) can be determined self-consistently from the constraint Eq.(9) and is given by

\[
\eta = |⟨b_0⟩|^2 = 2 - \frac{1}{N} \sum_k \frac{\xi_k}{\epsilon_k}. \tag{13}
\]

The minimum energy for charge excitation is given by \( \epsilon_{k=0} \). The Mott transition occurs when this gap closes. From this requirement, we find the \( U_c \) for Mott transition is given by \( U_c = 4ZJ \eta_c \). Here \( \eta_c \) is the value of \( \eta \) at which the gap closes and is given by

\[
\eta_c = 2 - \frac{1}{N} \sum_k \frac{1 - \gamma_k/2}{\sqrt{(1 - \gamma_k/2)^2 - \gamma_k^2}}. \tag{14}
\]

For a given lattice, \( \eta_c \) is a mathematical constant. On the triangular lattice, this constant is found to be \( \eta_c \approx 0.8971 \). Thus the \( U_c \) for the Mott transition on the triangular lattice is \( U_c \approx 3.5884K \approx 8.43t \). This is a better estimation than that obtained by the local mean field treatment we discussed above.\(^15\)

We now construct the variational wave function related to the new mean field theory. The mean field ground state of the system is the product of the paired ground state of \( b_1 \) and \( b_{-1} \) boson and the Fermi sea for the spinon,

\[
|\text{MF}⟩ = e^{\sum_i W(i,j) b_{i,1}^\dagger b_{j,-1}^\dagger}|0⟩|F - FS⟩, \tag{15}
\]

in which \( |0⟩ \) is the boson vacuum,

\[
W(i,j) = \frac{1}{N} \sum_k \frac{\Delta_k}{\xi_k + \epsilon_k} e^{ik·(R_i - R_j)}. \tag{16}
\]
is the pair wave function for the $b_{\pm 1}$ boson. In principle, we should also consider the condensate of the $b_0$ boson in the above mean field wave function. However, the $b_0$ condensate only contributes a multiplicative constant to the wave function, which only depends on the total number of singly occupied sites. Using the constraint Eq.(9), this multiplicative constant can be written in the form of a Gutzwiller factor $g^D$ and be absorbed in Eq.(15) by multiplying $W(i,j)$ with a factor $g$. The true electron wave function of the system is obtained by enforcing the rotor constraint Eq.(2) and is given by

$$|\Psi\rangle = \prod_i P_i |\Psi_{MF}\rangle = \text{Perm}[gW]|\Psi_{FS}\rangle.$$  \hspace{1cm} (17)

Here $|\Psi_{FS}\rangle$ is the Fermi sea state of the free electron, $\text{Perm}[gW]$ is the permanent of the matrix $gW$. $W$ is a matrix of dimension $D$ with its matrix element given by $W(i,j)$, which is the pair wave function between doubloon at site $i$ and holon at site $j$.

We have performed variational Monte Carlo study on the above wave function on the triangular lattice. As the computation of permanent of a matrix is exponentially expensive in its dimension, our calculation is limited to the large $U$ regime, when the number of doubloon is small. In our calculation, we have used a $12 \times 12$ cluster with periodic-antiperiodic boundary condition. There are two variational parameters, namely $g$ and $\lambda = \frac{U}{V^2 Z J^2}$, to be optimized in our wave function. To determine the $U_c$ for Mott transition, we use the mean field expression for the charge gap, which is given by $\epsilon_{\text{MF}} = \frac{U \sqrt{\lambda}}{2V} \sqrt{(\lambda - 1)^2 - 1}$. The gap closes when $\lambda$ approaches 2 from above. When $\lambda > 2$, the pair wave function $W(i,j)$ is short ranged and the holon and the doubloon are bounded together. Fig.1 plot the evolution of the charge gap with $U/t$. The gap exhibits a linear dependence on $U/t$ close to the Mott transition point. We note that the same behavior is also predicted by the large-N theory. From a linear extrapolation, we find the charge gap closes around $U/t \approx 10.75$. This result is higher than the generally accepted value of 7 to 8.

Finally, we compare our result with that produced by the wave function with long range Jastrow factor. The Jastrow wave function can be written as $|\Psi\rangle = e^{\sum_{i,j} v(i-j)n_i n_j} |\Psi_{FS}\rangle$. Here $n_i$ and $n_j$ denotes the electron number at site $i$ and site $j$, $v(i-j)$ is the variational parameter introduced to control the charge correlation between these two sites. The comparison of the ground state energies on a $12 \times 12$ lattice predicted by both theories is shown in Fig.2. For the Jastrow wave function, we have optimized the variational parameter $v(i-j)$ at all distances. The shoulder in the ground state energy around $U/t = 12$ is a precursor of the Mott transition in the thermodynamic limit. To see clearly the signature of Mott transition in the Jastrow wave function, much larger lattice is needed. Compared with the Jastrow wave function, the permanent wave function proposed in this paper is obviously better in the insulating phase, although it involves much smaller number of (only two) variational parameters.

In summary, we have proposed a new mean field theory for the Mott transition in the Hubbard model based on the slave rotor representation. The new theory can better capture the long range charge correlation, which is known to be crucial for a correct theory of Mott transition. The new theory predicts a continuous Mott transition on the triangular lattice around $U = 8.43t$ with non-divergent quasiparticle mass at the transition point. The variational wave function corresponding to the new mean field theory has the form of the product of the permanent for the charge degree of freedom and the determinant of the spin degree of freedom. The new wave function is found to work better than the fully optimized Jastrow wave function in the insulating phase. However,
the \( U_c \) predicted from such a wave function is still significantly larger than the generally accepted value. We think this deficiency should be attributed to the spin degree of freedom, for which the superexchange interaction in the large \( U \) regime is not fully accounted for by the Slater determinant wave function. It should be noted that such superexchange effect can be incorporated in the wave function through backflow correction in the Slater determinant.\(^{17,18}\) We find the backflow correction can indeed improve significantly the estimate of \( U_c \) in our wave function. A detailed discussion on this point is left as the subject of a future paper.

The computations have been done using the Magic-II Supercomputing facility in Shanghai supercomputing center, the RIKEN Integrated Cluster of Clusters (RICC) facility and the RIKEN supercomputer system (HOKUSAI Great Wave). Tao Li is supported by NSFC Grant No. 11034012 and Research Funds of Renmin University of China. This work has been also supported in part by RIKEN iTHES Project and Molecular Systems.

---

1. M. Imada, A. Fujimori, and Y. Tokura, Rev. Mod. Phys. 70, 1039 (1998).
2. Y. Shimizu, K. Miyagawa, K. Kanoda, M. Maesato and G. Saito, Phys. Rev. Lett. 91, 107001 (2003).
3. Y. Kurosaki, Y. Shimizu, K. Miyagawa, K. Kanoda, and G. Saito, Phys. Rev. Lett. 95, 177001 (2005).
4. T. Furukawa, K. Miyagawa, H. Taniguchi, R. Kato and K. Kanoda, Nature Physics 11, 221224 (2015).
5. O. I. Motrunich, Phys. Rev. B 72, 045105 (2005).
6. Z. Y. Meng, T. C. Lang, S. Wessel, F. F. Assaad, and A. Muramatsu, Nature 464, 847851 (2010).
7. S. Sorella, Y. Otsuka, and S. Yunoki, Sci. Rep. 2, 992 (2012).
8. M. Capello, F. Becca, M. Fabrizio, S. Sorella, and E. Tosatti Phys. Rev. Lett. 94, 026406 (2005).
9. B. O. Tayo and S. Sorella, Phys. Rev. B 78, 115117 (2008).
10. S. Florens and A. Georges, Phys. Rev. B 66, 165111 (2002).
11. S. Florens and A. Georges, Phys. Rev. B 70, 035114 (2004).
12. S. S. Lee and P. A. Lee, Phys. Rev. Lett. 95, 036403 (2005).
13. T. Senthil, Phys. Rev. B 78, 045109 (2008).
14. E. Zhao and A. Paramekanti, Phys. Rev. B 76, 195101 (2007).

In the large-N treatment, \( U_c \) is given by a similar expression of the form \( U_c = 4K/\beta^2 \), with \( \beta = \frac{1}{N} \sum_k \sqrt{1 - \gamma_k^2} \). On the triangular lattice, it predicts that \( U_c \approx 6.16t \). However, we note that the mean field prediction on \( U_c \) should not be taken too seriously, since correlation effect on the spin part and the entanglement between the charge and spin part are totally ignored in such treatment, which may shift \( U_c \) substantially.

The correlation between two holons (or two doublons) can be different from that between a holon and a doublon at short distance. A more accurate Jastrow wave function should take into account such a difference. However, we find the improvement in the ground state energy by such a change is much smaller than the energy difference between the Jastrow and permanent wave function.

15. L. F. Tocchio, F. Becca, A. Parola, and S. Sorella, Phys. Rev. B 78, 041101(R) (2008).
16. L. F. Tocchio, F. Becca, and C. Gros, Phys. Rev. B 83, 195138 (2011).