Order parameter for the Mott transition in two dimensions: Small-world network

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We show how to define the appropriate network measure that characterizes the nonmagnetic Mott transition starting from the Hubbard model on a square lattice. To simulate the Mott transition, we employ the variational Monte Carlo method based on the Gutzwiller wave function with nearest-neighbor doublon-holon binding correlations. In order to search the Mott transition point, we use the doublon-holon correlation function as the weighted network representation for analyzing the half-filled electronic system. We then show that a network quantity, small-worldness, can be applied to defining the order parameter describing a hidden "symmetry" broken in the network representation, which allows us to capture the Mott transition point. As a result, we suggest that the picture of the Mott transition can be obtained using a mass of data entirely contained in topologies of the proper weighted networks.

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Owing to the breakthrough in the control of ultracold atoms on optical lattices, Mott’s original ideas about metal-insulator transitions [1] have been realized in recent years [2,4]. His brilliant idea is well known as the Mott transition that a metal-insulator transition is driven by electron correlations. Although Mott insulators are usually related to antiferromagnetism, the Mott transition can also take place in the absence of long-range magnetic order. In the past years, much progress has been made from both theoretical and experimental sides in understanding Mott transitions [5]. A difficulty is the absence of the order parameter to characterize the critical behavior of the observables for the Mott transition not accompanied by the onset of antiferromagnetic order.

There are two earlier concepts as to what should be the order parameter to describe the physics around the Mott transition point from the metallic side. One is based on the disappearance of the Fermi liquid quasiparticles introduced by Brinkman and Rice [6]. However, the Brinkman-Rice transition actually exists only in infinite dimensions. Note that the Mott transition still can be characterized by the charge stiffness, which is the response to a twist, while no symmetry is broken here [7]. The other concept is that the metal-insulator transition can be viewed as a condensation of doubly occupied sites (doublons), namely, the reduction of the number of carriers in the insulating side [8]. For simplicity, we will use the latter idea to study the Mott transition, and also assume the trial wave function with only nearest-neighbor attractive correlations between a doublon and an empty site (holon) in variational calculations.

In general, phases can be distinguished using Landau’s approach, which characterizes phases in terms of underlying symmetries that are spontaneously broken. The information we need to understand phase transitions is encoded in appropriate correlation functions, e.g., the correlation length would diverge close to a quantum critical point. Particularly, the low-lying excitations and the long-distance behavior of the correlations near the critical phase are believed to be well described by a quantum field theory. A major problem is, however, that in some cases it is unclear how to entirely extract important information from the correlation functions if these states do not break any symmetries, such as the Mott transition.

In this letter, we propose the weighted network constructed by the correlation between a doublon and a holon to two-dimensional (2D) Hubbard model on a square lattice. Complex network theory has become one of the most powerful frameworks for understanding the network structures of many real systems [9,13]. According the graph theory, the elements of the system often are called nodes and the relationships between them, which a weight is associated with, are called links. Decades ago, this unnoticed idea constructing a weighted network from condensed matters had been proposed in quantum Hall systems [14]. However, we here define the link weight carrying important information as doublon-holon binding correlations in the Hubbard model.

In Fig. 1 one can see the network topologies corresponding to the metallic ($U = 0$) and insulating ($U = 12$) regimes (see the details in the following section). The weighted network of the insulating state exhibits that there are only few links with the strongest weight called “highways”, which looks very different from the metallic state. This observation reminds us of a well-known fact in real-world networks that the network with heterogeneous link distributions is resilient to random attacks or failures [15,16]. The robustness of the network from its heterogeneity seems to indicate a hidden “symmetry” in

FIG. 1: Network representations of 2D Hubbard model at interaction strength (a) $U = 0$ and (b) $U = 12$. The lattice size $N = 4 \times 4$. The thickness of links represents the magnitude of the doublon-holon correlation function. Color scale: Blue (Red) indicates the largest (smallest) link weights.
network space. More precisely, the symmetry describes a phenomenon that the network function and structure remain unchanged or invariant under random removal of its links. Thus it could allow us to define an order parameter in the Mott transition by using appropriate network measures.

The small-world network containing both strong clustering and shortest path length [17] has been considered to be a well-established fact in many real-world networks [18][21]. Recently the small-world idea has been successfully implemented in several statistical models as well [22]. In order to quantify the small-world network, we further propose a network quantity, small-worldness, as the order parameter in network space that would suddenly change while the Hubbard system undergoes a Mott transition. We find that it is able to extract the Mott transition point obtained by conventional quantities, such as charge stiffness. Based on this result as well as previous evidences obtained from different models [22], we suggest that the small-worldness can provide us another route to determine the order parameter in various many-body phase transitions represented by the network language.

**Model and method.**— We begin with the 2D half-filled Hubbard model on a square lattice, which is relevant to correlated electron materials [23]:

\[
H = \hat{H}_t + \hat{H}_U = -\sum_{\langle i,j \rangle, \sigma} \left( c_{i\sigma}^\dagger c_{j\sigma}^\ddagger + H.c. \right) + U \sum_i \hat{d}_i,
\]

where \( \hat{d}_i = n_{i\uparrow} n_{i\downarrow} \) and \( n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \) with spin \( \sigma \). In the following, we express the trial ground state in the finite system of \( N \) sites with (anti-)periodic boundary condition along the \( \hat{x} \) (\( \hat{y} \)) direction to satisfy the closed-shell condition.

For our numerical simulations, we use the variational Monte Carlo (VMC) approach, which is based on the well-known Gutzwiller wave function [24]:

\[
|\Psi_G \rangle = \hat{P}_G |\Psi_{FL} \rangle,
\]

where \( |\Psi_{FL} \rangle \) is the Fermi liquid and \( \hat{P}_G = g \sum_i \hat{d}_i \). Here \( g \) is the parameter to adjust the number of doublons in the system. However, it is impossible to realize the nonmagnetic Mott transition by just using \( |\Psi_G \rangle \). To demonstrate this transition, the simplest doublon-holon binding correlation must be considered [3][25].

\[
|\Psi_{DH} \rangle = \prod_i \left( 1 - \mu \hat{Q}_i \right) |\Psi_G \rangle,
\]

\[
\hat{Q}_i = \hat{d}_i \prod_\delta \left( 1 - \hat{h}_{i+\delta} \right) + \hat{h}_i \prod_\delta \left( 1 - \hat{d}_{i+\delta} \right).
\]

Here \( \hat{h}_i = (1 - n_{i\uparrow})(1 - n_{i\downarrow}) \) and \( \delta \) runs over the nearest neighbors of the site \( i \). \( \mu \) is the parameter to control the number of isolated doublons and holons. If \( \mu = 0 \), \(|\Psi_{DH} \rangle \) will be back to \(|\Psi_G \rangle \) which is metallic for \( U < \infty \). On the other side, \( \mu = 1 \), \(|\Psi_{DH} \rangle \) becomes a completely doublon-holon bound state that seems to be insulating. It has been numerically proven that \(|\Psi_{DH} \rangle \) is enough to describe the behavior of the Mott transition in VMC studies, even though we still need to consider more correlation factors to correctly capture the transition point [26]. Thus, it is reasonable to illustrate the occurrence of a nonmagnetic Mott transition by using the doublon-holon bound state \(|\Psi_{DH} \rangle \).

In the language of network analysis, each network of \( N \) nodes can be described by the \( N \times N \) adjacency matrix \( \hat{A} \). A number of real systems, e.g. social networks, transportation networks, biological networks and so on, are better captured by weighted networks in which links use the weight to quantify their strengths. Here we consider lattice sites as nodes of the weighted network of which each weighted link between nodes \( i \) and \( j \) is expressed by the element of the adjacency matrix \( \hat{A}_{ij} \). The link should carry the weight containing information about the relationship between electrons in the Hubbard system. According to the trial wave function we use, the weight of the network link is naively defined by the doublon-holon binding correlation.

Many of real networks have the property of relatively short average path length that is a shortest route running along the links of a network. In other words, most of nodes may not be neighbors but can reach each other by a small number of steps. This is called small-world phenomena [27]. However, the random networks showing the small-world effect fail to reproduce some important features of real networks, such as clustering. A small-world network including not only strong clustering but also short path length has thus been introduced to describe real networks by Watts and Strogatz [17]. Instead of the weighted clustering coefficient \( \langle c \rangle \) [28] and the average path length \( \langle d \rangle \) [29] commonly used in network analysis, an alternative measurement of the small-world property called “small-worldness” has been recently proposed [30]. The definition is based on the maximal tradeoff between high clustering and short path length. We can further define small-worldness as

\[
\langle s \rangle \equiv \frac{\langle c \rangle}{\langle d \rangle}.
\]

One can see much more details in Ref. [22]. A network with larger \( \langle s \rangle \) has a higher small-world level. Note that the small-worldness is appropriate to describing the universal critical properties as a result of the information about both locality (weighted clustering coefficient \( \langle c \rangle \)) and non-locality (average path length \( \langle d \rangle \)) in network space simultaneously included. In fact, we have shown that the small-worldness indeed can behave like an order parameter in either continuous or topological phase transitions in our previous works [22].

**Mott transition of physical observables.**—We now recall some facts about the nonmagnetic Mott transition arising from the doublon-holon binding effect [26]. The short-range doublon-holon binding correlation to describe the essence of the first-order Mott transition has been confirmed by several VMC calculations [31][32]. A recent VMC study also concludes that the size of the doublon-holon bound state in the insulating phase is not beyond the next nearest neighbors [26]. This result thus motivates us to simply consider the nearest-
neighborn doublon-holon binding correlation in the trial wave function $\Psi_{DH}$. However, the problem is that the proposals on the order parameter are still controversial even if the metal-insulator transition is well defined. In the following, we therefore examine several conventional physical observables to detect the critical point.

Figure 2(a) and (b) show the kinetic energy $E_t(\equiv \langle \hat{H}_t \rangle)$ and the interaction energy $E_U/U(\equiv \langle \hat{H}_U \rangle/U)$ which is substantially the doublon density. It is obvious that both the kinetic energy and the doublon density have a discontinuity at the critical point $U_c$ between 8.5 and 8.6, which has been indicated by the other VMC approach ($U_c = 8.575$) [26]. This is a typical sign of a first-order transition. Nevertheless, we cannot do anything but estimate the critical point from the maximum decreasing (minimum increasing) rate of the interaction energy $\partial E_U/\partial U$ (the kinetic energy $\partial E_t/\partial U$) if we want to precisely know where $U_c$ is.

To estimate the critical point more accurately, we need to consider other physical quantities. First, we start the charge density correlation function in momentum space called charge structure factor,

$$N_k = \frac{1}{N} \sum_{i,j} \langle n_i n_j \rangle e^{ik \cdot (R_i - R_j)} - n^2,$$

where $n_i = \sum\limits_\sigma n_{i\sigma}$ and $n$ electron density. One can see that the important information about the metal-insulator transition is concealed in the charge structure factor $N_k$. Within the variational theory, $N_k \propto |k|$ for $|k| \to 0$ if there is no charge gap, whereas $N_k \propto |k|^2$ if a charge gap opens. As illustrated in Fig 2(c), the momentum dependence of $N_k$ near the $\Gamma$ point abruptly changes between $U = 8$ and 9, which coincides with the critical region determined above. Even so, the way to distinguish the insulating phase from the metallic phase will need much more efforts on the interpolation between lattice points.

Then, we consider the momentum distribution function, $n_k = \sum\limits_\sigma \langle c^\dagger_{k\sigma} c_{k\sigma} \rangle$. According to Fermi liquid theory, the jump of $n_k$ near the Fermi surface, namely, the quasiparticle renormalization factor related to the charge stiffness, can be used to identify the metal-insulator transition. We show a clear discontinuity of $n_k$ around the Fermi surface for small $U$ in Fig 2(d), thus suggesting that it is the metallic phase. As further increasing $U$, the jump is evidently reduced and remains very small for large $U(> 9)$. The small residual value of the jump is basically due to the finite size effect. That means we need to make more endeavors to indicate the critical point $U_c$ estimated from the extrapolation to where the jump vanishes.

**Network analysis.**—Due to the doublon-holon binding effect leading to the nonmagnetic Mott transition, we can imagine that the correlation between a doublon and a holon provides a sufficient amount of data about the critical point $U_c$. Therefore, we define the doublon-holon correlation function as follows,

$$C_{dh}(R) = \frac{1}{N} \sum_i \langle \hat{d}_i \hat{h}_{i+R} \rangle.$$

In general, if a system shows the conventional long-range order, like ferromagnetism or crystal, the corresponding correlation function will be nonzero at its tail that can be used to define the order parameter. Otherwise, the correlation function would decay to zero at long distance for the system does not break any symmetry. Here it is very difficult to find the order parameter derived from the doublon-holon correlation because of unbroken symmetry in the nonmagnetic Mott transition.

In Fig 3 we show how the doublon-holon correlation function changes as the Mott transition occurs. For $U = 0$, no unusual relationship between a doublon and a holon would be observed in the Fermi-liquid ground state. As increasing $U$, a doublon starts to attract one holon at the nearest-neighbor site so that the doublon-holon correlation function $C_{dh}(R)$ is slowly enhanced only at $R = 1$. When $U$ is larger than the
critical value $U_c$, $C_{dh}(R)$ is rapidly increased at $R = 1$ as well as $C_{dh}(R = 1) \gg C_{dh}(R \neq 1)$ since the doublon-holon bound state begins to develop in the insulating phase. A key observation from Fig.3 is that while the system enters the insulating regime, the short-range parts of the doublon-holon correlation function rapidly decay with distances but the long-range parts still remain similar to the metallic phase. In order to search a possible order parameter in network space, we will take advantage of this property originating from different shapes of the correlation functions for different $U$.

We now investigate how the network techniques perform in the face of the metal-insulator transition. Based on the observation on the doublon-holon correlation, a straightforward definition for the elements of the adjacency matrix $\hat{A}_{ij}$ is the magnitude of the normalized doublon-holon correlation function between the lattice sites $i$ and $j$,

$$\hat{A}_{ij} = \frac{|\langle \hat{d}_i \hat{h}_j \rangle|}{\text{max}(\{|\langle \hat{d}_i \hat{h}_j \rangle|\})}. \quad (8)$$

The complex topology of the weighted network extracted from $\hat{A}_{ij}$ has been shown in Fig.4 for the small lattice. Obviously, the weight of network links exhibits different distributions for the metallic and insulating phases even though all nodes in the network are completely connected. It would be just a trivial complete network if the network were binary. Next, we need to collect the useful information from the large network data.

In our previous studies [23], we have confirmed that the small-worldness $\langle s \rangle$ defined in Eq.5 has the ability to detect the second-order and infinite-order phase transitions. Here we further examine the feasibility of the small-worldness in the first-order phase transition without any broken symmetries. In Fig.4(a), we illustrate the critical behavior of the small-worldness in the 2D Hubbard model. One can see that the $U$-dependence of the small-worldness behaves like an order parameter and drops down to almost zero around the critical point $U_c$ in the finite system of size $N = 16 \times 16$. In the inset of Fig.4(a), we find that the critical point is indicated by the sudden decrease of $\langle s \rangle$ between $U_c = 8.5$ and 8.6, which is in agreement with the results obtained above and in Ref.26. Note that the small-worldness for $U > U_c (~ 8.9)$ can be further reduced to zero in a larger lattice system ($N = 20 \times 20$). However, it is rather difficult to estimate $U_c$ by using finite-size calculations since the Mott critical value obtained from the doublon-holon binding wave function would become larger as increasing the system size. In any case, this agreement convinces us that the small-worldness can be used as another quantity to characterize the nonmagnetic Mott transition instead of the charge stiffness.

To understand the result that the small-worldness is quantitatively similar to an order parameter, we need to show how the weight distribution of the network link enables complex weighted networks to illustrate the phase transitions in many-body systems. Fig.4(b) shows that the weight of the network link displays two bounded distributions with the asymmetric bimodal shape. At $U = 0$, few links have the strongest weight ($W \sim 1$) from which the weights for most of links are not far away ($W \sim 0.75$). The bimodal shape is mainly due to the broken $C_4$ rotational symmetry by anti-periodic boundary condition along the $\hat{y}$ direction. Thus the weighted network for $U = 0$ possesses the most small-world property whose most of links resemble the highways in road networks.

We have to mention a point now in passing. In the network representation, there exists a kind of hidden “symmetry” corresponding to the heterogeneous network with a broad weight distribution. This symmetry is related to the robustness of the network that is the resilience to random attacks or failures. The heterogeneity of network links implies that the weighted network is more robust against attacks, giving rise to the higher symmetry in the network space. Conversely, the homogeneity of network links means that the weighted network becomes fragile to random attacks, and thus breaks the hidden symmetry. Therefore, if we ignored the bimodal shape arising from the anti-periodic boundary condition, the weighted network for $U = 0$ would exhibit the homogeneous weight distribution so that the hidden symmetry would be broken. We anticipate that the small-worldness carrying both local and non-local messages is able to represent the order parameter describing the broken symmetry in the network space.

As further increasing $U$, the weights for most of links begin to move away from 1 and the distributions show more heterogeneous, leading to the reduction of the small-worldness shown in Fig.4(a). When $U > U_c$, most of links have very small weights ($W \sim 0$) and few links with the strongest weight ($W \sim 1$) show the broader distributions. The phenomena that most of links are like slow traffic lanes result in almost zero small-worldness, namely, the broken “symmetry” in the network space is recovered due to the heterogeneity of network links. The same reasoning from the weight distribution of network links could be also applied to other many-body systems without local order parameters in real space. Hence this result strongly suggests that the small-worldness can be considered as a new order parameter in the network representation to capture the nonmagnetic Mott transition in the 2D
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Conclusions. In this work we have addressed how to read useful information from the doublon-holon correlation to identify the nonmagnetic Mott critical point by using complex network analysis. We have compared several conventional observables describing the Mott transition, and yet none of them can be formally treated as the order parameter. In the 2D Hubbard model, we have illustrated that one of many network measures, small-worldness, plays a significant role as an order parameter in network space relied on Landau symmetry-breaking theory. The critical point $U_c$ extracted from the small-worldness is very close to the one obtained from other physical observables.

The shifting and broadening of the weight distribution of network links across the critical point are responsible for the change of the small-worldliness, which is analogous to the change of the speed limit on a road network from the highway to the slow lane. The phenomenon that the structure of the weighted network varies from heterogeneity to homogeneity implies a hidden "symmetry" broken—or, to put it another way, the reduction of the robustness to random attacks in the network space. Also, the broken symmetry has been successfully described by the small-worldness. The weight distribution of network links is able to uncover a wealth of complex topological information underneath correlation functions, and further comprehends the mechanism of the phase transition without local order parameters in real space. As a result, it is expected that the small-worldliness determined from various weighted networks could be a valuable tool to investigate quantum phase transitions.

The findings have been corroborated by our previous results in the 1D quantum Ising and 2D classical XY models [22]. The evidence given in the 2D Hubbard model, one may conjecture that generally the point of view coming from complex network topology can be a vital component in studying the phase transitions in condensed matters. Yet some interesting questions remain open. For instance, it would be desirable to either search the weighted network in the interacting models with topological order or further examine the dynamics of the weighted network whose the links change as time progresses in many-particle systems. It is our hope that the present work will stimulate further studies in the future.

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[1] N. F. Mott, Metal-Insulator Transitions Taylor & Francis, London (1974).
[2] M. Greiner et al., Nature 415, 39 (2002).
[3] T. Stöferle, H. Moritz, C. Schori, M. Kohl, and T. Esslinger, Phys. Rev. Lett. 92, 130403 (2004).
[4] I. B. Spielman, W. D. Phillips, and J. V. Porto, Phys. Rev. Lett. 98, 080404 (2007).
[5] M. Imada, A. Fujimori, and Y. Tokura, Rev. Mod. Phys. 70, 1039 (1998).
[6] W. F. Brinkman and T. M. Rice, Phys. Rev. B 2, 4302 (1970).
[7] M. A. Continentino, Quantum Scaling in Many-Body Systems (World Scientific) (2001).
[8] C. Castellani, C. Di Castro, D. Feinberg, and J. Ranninger, Phys. Rev. Lett. 43, 1957 (1979).
[9] R. Albert and A.-L. Barabasi, Rev. Mod. Phys. 74, 47 (2002).
[10] S. N. Dorogovtsev and J. F. F. Mendes, Adv. Phys. 51, 1079 (2002).
[11] M. E. J. Newman, SIAM Rev. 45, 167 (2003).
[12] S. Boccaletti et al., Phys. Rep. 424, 175 (2006).
[13] S. N. Dorogovtsev, A. V. Goltsev and J. F. F. Mendes, Rev. Mod. Phys. 80, 1275 (2008).
[14] T. Senthil, J. B. Marston, and M. P. A. Fisher, Phys. Rev. B 60, 4245 (1999).
[15] R. Albert, H. Jeong, and A.-L. Barabasi, Nature 406, 378 (2000).
[16] B. Wang, H. Tang, C. Guo, and Z. Xiu, Physica A, 363, 591 (2006).
[17] D. J. Watts and S. H. Strogatz, Nature (London) 393, 440 (1998).
[18] R. Albert, H. Jeong and A.-L. Barabasi, Nature 401, 130 (1999).
[19] M. E. J. Newman, Proc. Natl. Acad. Sci. USA 98, 404 (2001).
[20] P. S. Dodds, R. Muhamad and D. J. Watts, Science 301, 827 (2003).
[21] L. Backstrom et al., Proceedings of the Third Annual ACM Web Science Conference (WebSci 2012) pp. 33 (2012).
[22] C.-P. Chou and M.-C. Chang, arXiv:1308.0255 (2013).
[23] F. Gebhard, The Mott Metal-Insulator Transition Models and Methods (Springer) (1997).
[24] M. Gutzwiller, Phys. Rev. Lett. 10, 159 (1963).
[25] H. Yokoyama, Prog. Theor. Phys. 108, 59 (2002).
[26] T. Miyagawa and H. Yokoyama, J. Phys. Soc. Jpn. 80, 084705 (2011).
[27] D. J. Watts, Small worlds: the dynamics of networks between order and randomness, Princeton University Press (1999).
[28] J. P. Onnela, J. Saramaki, J. Kertesz and K. Kaski, Phys. Rev. E 71, 065103 (2005).
[29] M. E. J. Newman, Networks: an introduction, Oxford University Press (2010).
[30] M. D. Humphries and K. Gurney, PLoS ONE 3, e0002051 (2008).
[31] H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. 59, 3669 (1990).
[32] H. Yokoyama, Y. Tanaka, M. Ogata, and H. Tsuchiura, J. Phys. Soc. Jpn. 73, 1119 (2004).