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Doublon–holon-binding mechanism of Mott transition in 2D Hubbard model

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ABSTRACT

The mechanism of nonmagnetic Mott transitions in the Hubbard model on the square lattice is studied, using a variational Monte Carlo method. A simple doublon (D)–holon (H) binding mechanism a previous study proposed [J. Phys. Soc. Jpn. 75 (2006) 114706] has to be modified, because even a wave function with completely bound D–H pairs brings about a Mott transition at a finite correlation strength. By introducing two characteristic lengths, D–H pair binding length, ξ_{DH}, and minimum inter-doublon distance, ξ_{DD}, we can properly describe the physics of Mott transitions, and determine the critical point by $\xi_{DD} \sim \xi_{DH}$. This concept seems universal, because it is valid not only for newly introduced wave functions with long-range D–H and D–D (H–H) correlation factors discussed here, but for a wide range of wave functions with D–H binding factors.

1. Introduction

In connection with the cuprate superconductors, which are known as so-called doped Mott insulators [1,2], it is vital to understand the mechanism of Mott transitions. In this work, through a variational Monte Carlo (VMC) approach, we address this phenomenon in the single-band Hubbard model on the square lattice:

$$\mathcal{H} = -t\sum_{\langle i,j\rangle\sigma}(c^{\dagger}_{i\sigma}c_{j\sigma} + h.c.) + U\sum_{j} n_j n_j, \tag{1}$$

where the notation is standard ($t, U \geqslant 0$). Although it is certain for fermions that metal–insulator transitions occur at $U/t = 0$ in this model on hypercubic lattices, the transitions are of magnetic origin owing to the good nesting conditions [3]. This point is corroborated by comparing with the spinless ($S = 0$) Bose Hubbard models on hypercubic lattices, which exhibit superfluid-insulator transitions at finite values of U/t related to the band width of corresponding fermionic models [4]. Here, we study the Mott transition without any magnetic order in its original sense, namely, a transition arising owing to the competition between the kinetic and interaction energies. In this line of variation theory, it is known that the Gutzwiller wave function [5], with only onsite correlation factor, is always metallic, and by itself do not exhibit a Mott transition at finite U/t for fermions [6]. In previous papers [7,8], however, the authors showed that first-order Mott transitions actually occur at U/t roughly of the band width in wave functions with an attractive correlation factor between a doubly occupied site (doublon, D) and an adjacent empty site (holon, H) [9,10], and argued that the binding of a doublon (minus charge carrier) to a holon (plus charge carrier) and the unbinding play the central role in the Mott transition [8]. In this picture, a doublon simply dissociates from a holon in the metallic side of the critical point, U_c/t; consequently, a doublon and a holon, namely carriers, can move about independently.

Later on, we have found that Mott transitions occur even in wave functions in which a doublon must be necessarily accompanied by at least one holon in the nearest-neighbor (NN) sites. Namely, the state in which a doublon and a holon always tightly bind one another can be metallic. This finding requires a modification of the previous picture of Mott transitions through D–H binding and simple release [8].

The purpose of this article is to briefly describe an improvement over the previous D–H binding picture, on the basis of VMC calculations. To begin with, we study the Mott transition arising in the completely D–H bound state on the square lattice, which affords a clue to a new conception. Then, we introduce two characteristic lengths, the D–H pair binding length ξ_{DH} and the mutual doublon exclusive distance ξ_{DD}. ξ_{DH} roughly represents the size of a D–H pair, and ξ_{DD} the minimum distance between two doublons. Generally, the two lengths depend largely on U/t. In the metallic phase, a relation $\xi_{DH} > \xi_{DD}$ holds, whereas in the insulating phase, the relation is reversed. Thus, a Mott transition occurs at a value of U/t, where ξ_{DD} becomes equivalent to ξ_{DH}. By checking a variety of wave functions, including newly introduced one with long-range Jastrow factors, we are convinced that this conception is applicable to a wide range of systems, including Bose Hubbard models [4].

2. Formulation

To tackle the Mott physics, we apply a VMC method to the single-band Hubbard model (Eq. (1)) at half filling on the square

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lattice. The VMC method is one of few effective approaches to the Mott transition, because this method can deal with the strong local correlation accurately, and thereby, systems in the whole range of correlation strength can be treated continuously. Here, we concentrate on a few fundamental wave functions to capture the essence:

$$|\psi_G\rangle = \mathcal{P}_G\,|\phi_F\rangle, \tag{2}$$

$$|\psi_B\rangle = \mathcal{P}_B^{d-h}\mathcal{P}_G\,|\phi_F\rangle, \tag{3}$$

$$|\psi_{pow}\rangle = \mathcal{P}_{pow}^{d-h}\mathcal{P}_{pow}^{d-d}\,|\phi_F\rangle, \tag{4}$$

where $|\phi_F\rangle$ denotes the Fermi sea. Eq. (2) is the celebrated Gutzwiller wave function [4], which adjusts the doublon density by an on-site correlation parameter g:

$$\mathcal{P}_G = \prod_j [1-(1-g)n_j n_j]. \tag{5}$$

Because $|\psi_G\rangle$ is always metallic as far as U/t is finite [6], we refer to $|\psi_G\rangle$ for a typical metallic state. In Eq. (3), $\mathcal{P}_B^{d-h}$ is written as,

$$\mathcal{P}_B^{d-h} = \prod_j \left\{1-\left[d_j\prod_{\vec{\tau}}(1-h_{j+\vec{\tau}})+h_j\prod_{\vec{\tau}}(1-d_{j+\vec{\tau}})\right]\right\}, \tag{6}$$

where $d_j = n^j n_j$ and $h_j = (1-n^j)(1-n_j)$ are doublon and holon operators respectively, and $\vec{\tau}$ varies over the four NN sites of the site j. $|\psi_B\rangle$ is an extreme case of the D–H binding wave function within the NN sites [9,10]; the projector $\mathcal{P}_B^{d-h}$, which has no adjustable parameter, returns 1 or 0, according as at least one H (D) exists in the four NN sites of each and every D (H) site or not. Thus, $|\psi_B\rangle$ represents a state in which D (H) must contact H (D) in the NN sites, that is, a completely D–H bound state, seemingly insulating. Although $|\psi_B\rangle$ is always insulating in a one-dimensional chain [11], $|\psi_B\rangle$ is not necessarily insulating in the square lattice, as we will discuss later. In Eq. (4), we consider long-range Jastrow-type correlation factors; the projectors are formally written as,

$$\mathcal{P}_{pow}^{d-h} = \prod_j \left(f_{dh}(\tilde{r}_j)\left\{d_j\left[1-\prod_{\tilde{r}_j}(1-h_{j+\tilde{r}_j})\right]+h_j\left[1-\prod_{\tilde{r}_j}(1-d_{j+\tilde{r}_j})\right]\right\}\right) \tag{7}$$

$$\mathcal{P}_{pow}^{d-h} = \prod_j \left(f_{dd}(\tilde{r}_j)\left\{d_j\left[1-\prod_{\tilde{r}_j}(1-d_{j+\tilde{r}_j})\right]+h_j\left[1-\prod_{\tilde{r}_j}(1-h_{j+\tilde{r}_j})\right]\right\}\right) \tag{8}$$

where the index j of the outside product varies over all the lattice sites. In Eq. (7), for a certain j, we count only in the case of the shortest D-to-H distance (for the first term in the braces) or of the shortest H-to-D distance (for the second term). This restriction as to distance is symbolically expressed by tilde ($\tilde{r}_j$). The index $\tilde{r}_j$ in the inside product varies over all the sites of distance r_j from the site j. To measure the distance, we adopt the stepwise or "Manhattan" metric in unit of lattice constant. A similar regulation is applied to Eq. (8). The function $f_{dh}(\tilde{r}_j)$ [$f_{dd}(\tilde{r}_j)$] works as the weight of distance-dependent D–H attractive [D–D and H–H repulsive] correlation. Among a wide choice of their forms, we focus on power-law decaying types in this work: $f_{dh}(\tilde{r}_j) = \tilde{r}_j^{-\xi}$ and $(f_{dd}(\tilde{r}_j) = 1-\alpha\tilde{r}_j^{-\beta}$, because they are simple to deal with and energetically favorable in some degree. In the attractive projector $\mathcal{P}_{pow}^{d-h}$, ξ in $f_{dh}(\tilde{r}_j)$ is a parameter controlling the D–H binding length; for $\xi = 0$, the D–H binding effect vanishes, whereas for $\xi = \infty$, $\mathcal{P}_{pow}^{d-h}$, is reduced to the NN binding projector $\mathcal{P}_B^{d-h}$. In the repulsive projector $\mathcal{P}_{pow}^{d-h}$, the parameter α controls the magnitude of repulsive factor in the NN sites; and β adjusts the effective distance of repulsion. Finally, we point out that in the study of Mott transitions, the attractive (D–H) and repulsive (D–D and H–H) Jastrow factors should be independently parameterized, because the roles of the two factors are distinct against this phenomenon. The D–H factor is crucial. In this point, the present factor $\mathcal{P}_{pow}^{d-h}\mathcal{P}_{pow}^{d-d}$ in Eq. (4) is distinguished from that in previous studies [12,13].

In VMC calculations, we use systems of $N_S(=L\times L)$ sites, and impose the boundary conditions periodic in the x direction and antiperiodic in the y direction (periodic-antiperiodic boundary conditions). For each wave function of Eqs. (2)–(4), we first minimize the energy and obtain a set of optimized variational parameters, using a quasi Newton method with recently derived relations [14] to treat Jastrow factors. Typically, we use the averages of 20 iterations converged, with 250,000 samples for each iteration. Then, physical quantities are calculated with the optimized parameter set.

3. Results

We start with the comparison of minimized total energy per site E_{tot}/t. In Fig. 1, the VMC estimates of E_{tot}/t are compared among the three wave functions, Eqs. (2)–(4). The long-range D–H binding state $|\psi_{pow}\rangle$, which includes $|\psi_G\rangle$ and $|\psi_B\rangle$ as extreme cases, is, of course, the lowest for any U/t, but the improvements on $|\psi_G\rangle$ for small U/t and on $|\psi_B\rangle$ for large U/t are slight. For a metallic state with small U/t, the D–H binding effect is little advantageous, and $|\psi_{pow}\rangle$ represents a typical metallic state. On the other hand, the D–H completely bound state $|\psi_B\rangle$ represents an insulating state for U sufficiently larger than the band width, W (=8t); thus, $|\psi_{pow}\rangle$ also represents an insulating state there. This is supported by the behavior of $E_{tot}/t \propto -t/U$ for $U/t\to\infty$, as shown in Fig. 1. Hence, $|\psi_{pow}\rangle$ should exhibits a metal to insulator transition at $U\sim W$, similarly to the adjacent D–H binding wave function ($U_c/t = 8.6$—8.7) [8]. To specify the critical value U_c/t for $|\psi_{pow}\rangle$, we consider the doublon density, $\langle D\rangle = \frac{1}{N_S}\sum_i\langle d_i\rangle$, which is an important quantity as an order parameter of Mott transitions, and proportional to the onsite charge fluctuation. As shown in Fig. 2, the behavior of $\langle D\rangle$ for $|\psi_{pow}$ abruptly changes at $U/t\sim 8.4$; for $U/t > 8.4$, it rapidly approaches that for $|\psi_{pow}\rangle$. Thus, we conclude that a Mott transition occurs at $U_c/t = 8.3\sim 8.5$ for $|\psi_{pow}\rangle$ of $L = 16$,

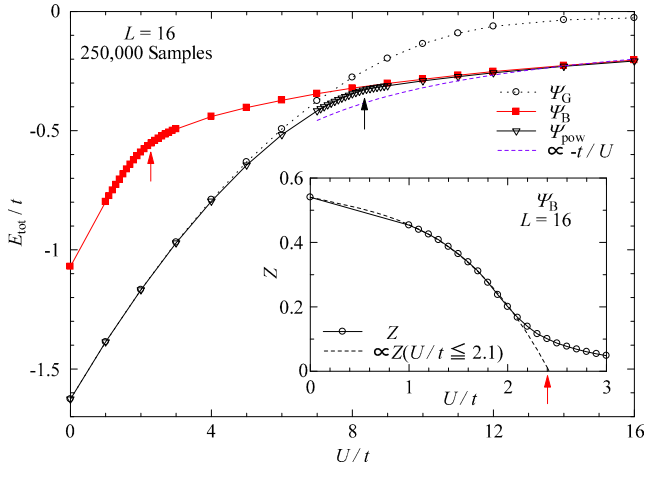

Fig. 1. Comparison of optimized variational energies among three trial wave functions, namely, Gutzwiller wave function $|\psi_G\rangle$, open circle), one with completely-bound D–H correlation ($|\psi_B\rangle$, solid square) and one with long-range Jastrow-type factors ($|\psi_{pow}\rangle$, open triangle), as function of correlation strength. The arrows on the curves indicate the Mott critical point. The dashed line is a guide line proportional to t/U expected from the strong-coupling expansion. The inset shows the quasiparticle renormalization factor as a function of U/t. We extrapolate Z to zero, indicated by an arrow, with the third-order least-square method from the data for $U/t\le 2.1$.