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Variational study of Mott transition by means of Drude weight and superfluid density

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Abstract

To distinguish a metal from an insulator, the Drude weight ($D$, zero-frequency component of conductivity) is a useful measure, as Kohn pointed out long ago: $D > 0$ (0) for a metal (insulator). Later, Millis and Coppersmith showed that a variational wave function $\Psi$ in which the key ingredient for a Mott transition (a doublon-holon binding effect) is introduced exhibits $D > 0$ (metallic) even for sufficiently large correlation strength, namely, a Mott transition is absent from $\Psi$. In contrast, variational Monte Carlo studies using $\Psi$ confirmed, by studying relevant quantities such as doublon density $d$ and a superconducting correlation function $\Psi$, that $\Psi$ doubtlessly raises a Mott transition. This contradiction has been a long-standing perplexing problem. We definitely settle this problem by adding to $\Psi$ a configuration-dependent phase factor $\Theta$ that has been hitherto overlooked. This factor appropriately picks out a negative counterpart in $D$ for insulators, so that $D$ vanishes. Because $\Theta$ does not affect the quantities such as $d$ and $\Psi$, the previous results on the Mott transition remain intact for $\Psi$.

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1. Introduction

Recently, “Mott physics” [1] returned to an active subject, thanks to the ultracold atoms on optical lattices and the application called “Mottronics”, besides cuprate and organic superconductors (SC) as (doped) Mott insulators. To support such experimental progress, it is urgent to establish the fundamentals of Mott physics using a reliable non-perturbative approach which continuously connects the weak- and strong-correlation limits, such as the dynamical mean field approximation and a variational Monte Carlo (VMC) method. Nearly half a century ago, Kohn introduced a useful criterion for discriminating between a metal and an insulator [2], namely, the Drude weight ($D$) is finite (zero) in a conductive (insulating) phase. The Drude weight is calculated as $D = \frac{d^2 E(A)/dA^2}{[2]}$ by introducing a virtual flux (Peierls phase) $\phi$ or by twisting the boundary condition. This formalism is advantageous to the VMC method, because $D$ can be calculated only from the information at $T = 0$. Later, Millis and Coppersmith [3] calculated $D$ for the one-dimensional Hubbard model, using a wave function $\Psi$ which includes a binding effect between a doubly occupied site (doublon, D) and an empty site (holon, H) [4] and is promising for bringing about a Mott transition. They found, however, that $D$ remains positive (actually the absolute value of kinetic energy) for a considerably large correlation strength $U/t$, and concluded that $\Psi$ is insufficient to describe a Mott transition. Their work (and Ref. [4]) caused misunderstanding to followers [5,6]. In fact, a number of VMC studies in a variety of situations [7-11] found within the scope of $\Psi$ that distinct Mott (or corresponding) transitions are confirmed at $U \sim W$ ($W$: bandwidth), where most physical quantities exhibit sharp anomalies (discontinuities, cusp, etc.). This inconsistency has long been a perplexing problem to be resolved.

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In this work, we settle this problem definitely, namely, the inconsistent behaviour of $D$ in the Mott insulating phase is reconciled by adding a configuration-dependent phase factor $P\psi_Q$ to $\Psi_Q$. In Sec. 2, we explain the details of trial wave functions to estimate the Drude weight using Kohn’s formula, and mention why $\Psi_Q$ fails in yielding an appropriate $D$. In Sec. 3, we give the results of VMC calculations using $P\psi_Q$. In Sec. 4, we briefly summarize and discuss our results.

2. Method

As a basic model which captures the essence of the Mott transition, we consider the Hubbard model on the square lattice for $U, t \geq 0$:
\[ H = H_t + H_0 = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_j d_j, \]
with $d_j = n_{j\uparrow} n_{j\downarrow}$. Because this model entirely satisfies the nesting condition at half filling ($n = N_e/N = 1$, $N_e$: electron number, $N$: site number), the ground state is an antiferromagnetic (AFM) or Slater insulator with a long-range order for $U > 0$. However, it is known for a large $U/t$ that the AFM order is incidental to the Mott insulating state, and our interest here is nonmagnetic Mott transitions on general lattices; we restrict our discussion to the nonmagnetic sector. To Eq. (1), we take a VMC approach. As a trial wave function, we adopt a two-body Jastrow form, $\Phi_Q = P\Phi$, where $P$ is a many-body correlation factor and $\Phi$ is a one-body part, for which we consider a normal state (Fermi sea) $\Phi_F = \Pi_{k\neq k_0, \sigma} \phi_{k\sigma}^\dagger \phi_{k\sigma}$ (vac) and a superconducting (SC) state ($d$-wave BCS state)

\[ \Phi_d = \left( \sum_k a_k c_{k\sigma}^\dagger c_{-k\sigma}^\dagger \right)^{N_e/2} \left( \text{vac} \right) \]
with $a_k = \frac{\Delta_d(k)}{\epsilon_k - \xi + \sqrt{\epsilon_k - \xi^2 + |\Delta_d(k)|^2}}$, ($\Delta_d(k)$ and $\Delta_d(k)$ represents the binding between a doublon (doubly occupied site) and its nearest-neighbor (NN) holon (unoccupied site) [4]. $Q_j$ is explicitly given by $Q_j = \mu_d d_j \sum_i (1 - h_{j+i}) + \mu_h h_j \sum_i (1 - h_{j+i}) (0 \leq \mu_d, \mu_h \leq 1)$ where $h_j = (1 - n_{j\uparrow})(1 - n_{j\downarrow})$, and $\tau$ runs over the NN sites of site $j$. This type of wave function brings about a Mott transition at $U\sim W$ as previous studies clarified [7-11], but does not yield a correct Drude weight [3].

Now, we explain how to calculate $D$, the zero-frequency component of conductivity $\sigma(\omega) = \pi D \delta(\omega) + \sigma^{\text{reg}}(\omega)$. $D$ is often estimated using the linear response theory, while Kohn [2] proposed another convenient formulation. According to it, $D$ is represented by the energy increment when a virtual potential vector (A) is applied to the system as a Peierls field as follows:

\[ H(A) = -t \sum_{\langle i,j \rangle, \sigma} \left[ e^{iA(\tau_i - \tau_j)} c_{i\sigma}^\dagger c_{j\sigma} + e^{iA(\tau_i - \tau_j)} c_{j\sigma}^\dagger c_{i\sigma} \right] + U \sum_j n_{j\uparrow} n_{j\downarrow}. \]

By writing the ground state of this Hamiltonian as $|A\rangle$, the Drude weight is given by $D = \frac{d^2 E(A)}{dA^2}$ for $A \rightarrow 0$, where $E(A) = \langle A|H(A)|A\rangle$. The vector potential is taken in the x direction ($A = Ax$). According to this formula, $E(A)$ is quadratic in $A$ (constant), if the system is metallic (insulating). Because only the ground state is involved in this formulation, it is suitable for a VMC method.

To grasp why $D$ obtained with conventional $\Psi_Q$ does not vanish in the insulating regime ($U > U_c$), let us transform Kohn’s formula using Hellmann-Feynman’s theorem and Eq. (3) to

\[ D = \left. \frac{d^2 E(A)}{dA^2} \right|_{A=0} = \left. \left[ \frac{d^2 H}{dA^2} \right]_{A=0} \right| + \left. \left[ 2 \left( \frac{dH}{dA} \right) \frac{d}{dA} \left| A \right| \right]_{A=0} \right| - \left. \left( [A] \right) \right|_{A=0}.
\]

Because the first term is equivalent to the $x$-direction kinetic energy of inverse sign, $-(H_t/2)$, which is the frequency sum of the optical conductivity and is positive, the second term must be a negative counterpart, if $D$ vanishes. Note that the second term has the imaginary unit $i$; therefore, $|A\rangle$ must have a phase factor related with $A$, if the second term has a finite contribution. It follows that $D = -(H_t/2)$ holds, if the trial wave function is real, as in the case of $\Psi_Q$. Actually, we can confirm $D = -(H_t/2)$ for $\Psi_Q$ [3]. Thus, in terms of the Drude weight, $\Psi_Q$ is metallic as far as $U/t < \infty$. Now, we are aware that we need to extend the trial wave function to a complex plane. This is reasonable, because the Hamiltonian for $A > 0$ [Eq. (3)] is essentially complex.

It is not difficult to construct a primitive phase factor which satisfies the above requirements for $U > U_c$. When an electron hops to the $x$ ($-x$) direction in Eq. (3), a phase $e^{iA}$ ($e^{-iA}$) is added to the expectation value $\langle H(A) \rangle$. This phase can be cancelled, the energy will not increase with $A$, namely $E(A) = E(0)$. In the Mott insulating regime, it is known [12] that the hopping processes in which doublon-holon pairs are created or destroyed predominantly
contribute to the kinetic energy. Namely, an electron hops rightward (leftward), if a doublon is located in the left-hand (right-hand) side of a holon in the initial configuration, as shown in Fig. 1. Accordingly, it is reasonable to add a phase factor \( e^{i\theta} \) \( \left( e^{-i\theta} \right) \) to the left-hand (right-hand) side local configuration in Fig. 1, where \( \theta \) is a new variational parameter. As for the doublon-creation processes, a parallel discussion holds with respect to the final configurations. We can explicitly write this configuration-dependent phase factor in a simple form as

\[
P_\theta = \exp \left[ i\theta \sum_j d_j (h_{j+1} - h_{j-1}) \right].
\]

(5)

In this study, we apply \( \Psi_\theta = P_\theta P_Q P_G |\Phi\rangle \) to Eq. (3) for estimating \( D \) from Kohn’s formula. If \( \Psi_\theta \) is optimized at \( \theta = A \), \( D \) is expected to vanish. It is important to notice that \( \Psi_\theta \) is optimized at \( \theta = 0 \) for \( A = 0 \), namely, \( \Psi_\theta \rightarrow P_Q P_G |\Phi\rangle \). Consequently, the results of quantities other than \( D \) obtained in the previous studies using \( \Psi_Q \) \{7-11\} remain intact. For a pairing (SC) state such as \( \Psi_d = P_\theta P_Q P_G |\Phi_d\rangle \), \( D \) becomes equivalent to the superfluid density \( D_s \) \{13\}.

In the VMC calculations, we use a quasi-Newton algorithm for the optimization, using substantially several million samples for the systems of \( N = L \times L \) sites with \( L = 12 \) and some electron densities \( n = 0.75-1.0 \) with the periodic-antiperiodic boundary conditions. The results for \( L = 16 \) only make small quantitative differences.

3. Results

We start with the \( A \) dependence of energy increment at half filling. For \( U = 0 \), the energy per site is given by \( E(A) = E(0) \cos A \), resulting in \( E(A) - E(0) \propto A^2 \) for \( A \to 0 \). This quadratic behaviour continues for small values of \( U/t \), as shown in Fig. 2(a) for the \( d \)-wave state. Thus, in this regime, the state is considered to be metallic. For large values of \( U/t \), however, \( E(A) - E(0) \) becomes constant for \( A \to 0 \), in contrast with the case for \( \Psi_Q \) \{3\}. Actually, it is known in \( \Psi_Q \) \{8\} that a Mott transition (first order in most cases) occurs at \( U_c / t \sim 6.5 \). Thus, the Drude weight should change from finite to zero at \( U = U_c \). To elucidate this point, we consider the optimized phase parameter \( \theta \) in \( P_\theta \). Shown in Fig. 2(b) is the \( U/t \) dependence of \( \theta / A \), where \( A \) is fixed at 0.4 \( \pi / L \). As \( U/t \) increases, \( \theta / A \) increases but remains sufficiently smaller than unity for \( U/t < 6.5 \). At \( U/t \sim 6.5 \), \( \theta / A \) shows a sudden discontinuous increase and reaches nearly unity, which value is preserved for larger \( U/t \). This singular point for \( \theta / A (A \to 0) \) is in complete agreement with the Mott transition point \( U_c / t \) determined by various quantities in \( \Psi_Q \). Thus, the Peierls phase \( A \) is cancelled out by \( \theta \) for \( U > U_c \), and the energy does not increase even if \( A \) is applied.

![Fig. 2. (a) Energy increment per site, \( E(A) - E(0) \), at half filling as a function of vector potential for some values of \( U/t \). (b) Optimized Variational parameter \( \theta \) normalized by vector potential \( A \). The data of both figures are for the \( d \)-wave pairing state, \( \Psi_d \).](image_url)

Now, let us discuss the Drude weight \( D \) (or \( D_s \)) estimated for \( \Psi_d \) and \( \Psi_F = P_\theta P_Q P_G |\Phi_F\rangle \). Figure 3(a) shows \( D \) (or \( D_s \)) in \( \Psi_d \) for some electron densities \( n \). At half filling (\( n = 1 \)), as \( U/t \) increases, \( D \) decreases from \( |E_t / 2t| \) for \( U = 0 \), drops to nearly zero at \( U_c / t \), and substantially vanishes for \( U > U_c \). Thus, we first succeeded in addressing a Mott transition and a Mott insulator by means of the Drude weight in a variation theory. The transition seems the first order, consistent with former results in \( \Psi_Q \) \{7-11\}. As the electron density decreases or the doping rate \( \delta (= 1 - n) \) increases, \( D \) monotonically increases for \( U > U_c \). In Fig. 3(b), the \( \delta \) dependence of \( D \) is shown for four values of \( U/t \). The behaviour for \( U > U_c \) is linear in \( \delta \), which is consistent with the results of the exact diagonalization \{14\}, VMC method based on the \( t-J \) model \{5\}, and experiments for cuprate superconductors \{15\}. Thus, the doped holes are relevant to the DC conductivity for \( U > U_c \); this is consistent with the picture of the doped Mott insulator \{1\}.
In contrast, for $U < U_c$, $D$ is finite at half filling, and changes only slightly as a function of $\delta$, as shown in Figs. 3(a) and 3(b). In this regime, it is appropriate to consider that the carriers are electrons as in the conventional Fermi liquid or BCS theory, where the Fermi-liquid behaviour, $D \sim (1 - \delta)/m^*$ ($m^*$: effective mass), may be applied.

As shown in Figs. 3(c) and 3(d), the difference between the SC and normal states is small except for $U \sim U_c$, where the behaviour is somewhat different between $\Psi_d$ and $\Psi_f$ [7,8]. This overall similarity indicates that the basic mechanism of DC conduction as doped Mott insulators do not depend on the details of the states.

4. Summary and discussions

We showed that, on the basis of Kohn’s formalism [2], the Drude weight or superfluid density can be appropriately calculated using a variation theory, and they vanish in the Mott insulating regime. Namely, the long standing problem of Millis and Coppersmith [3] was solved. The key to this success is the addition of a configuration-dependent phase parameter $P_0$ in Eq. (5). The $D_S$ calculated in the underdoped regime is consistent with the so-called Uemura plot [15] for cuprates, indicating that $P_0$ appropriately works also for the doped Mott insulators.

The simple factor $P_0$ is suitable for $U > U_c$, where the patterns of hopping are limited, whereas, for $U < U_c$, more refined phase factors are desirable, because there exist diverse hopping patterns. Another improvement will be achieved by modifying the one body part. In this connection, Scalapino et al. [13] showed with a mean-field treatment that $D$ vanishes for $n = 1$ and $U/t \to 0$ in the spin density wave state, in contrast to the normal and SC states. In this case (band insulator), the first-order-perturbed wave function for $\Phi$ is crucial in introducing a corrective phase. A full description of this study will be published elsewhere.

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