Finite-Temperature Signatures of Spin Liquids in Frustrated Hubbard Model

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Finite-temperature properties of the frustrated Hubbard model are theoretically examined by using the recently proposed thermal pure quantum state, which is an unbiased numerical method for finite-temperature calculations. By performing systematic calculations for the frustrated Hubbard model, we show that the geometrical frustration controls the characteristic energy scale of the metal-insulator transitions. We also find that entropy remains large even at moderately high temperature around the region where the quantum spin liquid is expected to appear at zero temperature. We propose that this is a useful criterion whether the target systems have a chance to be the quantum spin liquid or the non-magnetic insulator at zero temperature.

Introduction.– Strong correlations among particles often induce localization of the particles and resultant charge-gapped states are called Mott insulators. The Mott insulators have been ubiquitously found in a broad range of condensed matter physics [1–3]. In most of the Mott insulators in solids, time-reversal symmetry-broken phases such as antiferromagnetic phases appear at sufficiently low temperatures. However, if geometrical frustration becomes large [4], the quantum melting of the magnetic orders leads to new states of matter such as quantum spin liquids (QSL) [5, 6]. Actually, in the several organic conductors, it has been pointed out that QSL appear [7–9]. It has been one of the hottest issues of the modern condensed matter physics to clarify how the interplay of strong electronic correlations and the geometrical frustrations induces the QSL [10].

The two-dimensional Hubbard model with geometrical frustrations, which has the nearest-neighbor [nn] (next-nearest-neighbor [nnn]) hopping $t$ ($t'$) and on-site Coulomb interaction $U$ (details are defined in Eq. (1) later) is one of the simplest theoretical models that describes interplay between the strong electronic correlations and the geometrical frustrations. In this model, due to $t'$, which induces the nnn antiferromagnetic interactions, as illustrated in the inset of Fig. 1, the competition between two magnetic phases occurs: a simple Néel state becomes stable for small $t'$ while a stripe state becomes stable for large $t'$ region ($t'/t \sim 1$). Several theoretical calculations for the ground states of the frustrated Hubbard model [11–13] and its strong coupling limit $J_1$-$J_2$ Heisenberg model ($J_1 \sim 4t^2/U$, $J_2 \sim 4t'^2/U$) [14, 17] have been done thus far and most of the calculations suggest that QSL states appear around the intermediate region. In spite of the huge amount of the studies on the frustrated Hubbard model and $J_1$-$J_2$ Heisenberg model, there are few unbiased theoretical studies on the finite-temperature properties that are accessible in experiments because of a lack of efficient theoretical methods.

In this Letter, by using an efficient unbiased numerical method, i.e., the thermal pure quantum (TPQ) method [18], we systematically study finite-temperature properties of the frustrated Hubbard model, which is a prototypical system where the competition between the geometrical frustrations and the strong electronic correlations plays a crucial role. From the unbiased and systematic calculations, we clarify how the geometrical frustrations controls the crossover temperatures of the Mott transitions and find the finite-temperature signatures of QSL. We also propose an experimental criterion of closeness to the spin liquid phase: Finite-temperature entropy at moderately high temperatures significantly correlates with closeness to the spin liquid phase. Experimental searches for spin liquids have so far focused on setting up an alibi of spontaneous symmetry breakings down to ultra-low temperatures. However, we reveal that, even at moderately high temperatures $T\sim t/10$, it becomes clear whether the target system has chance to be a spin liquid at zero temperature.

Model and Methods.– We study the $t$-$t'$ Hubbard model on a square lattice (see Fig. 1) defined as

$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) - t' \sum_{\langle\langle i,j \rangle\rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow},$$

(1)

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) is a creation (annihilation) operator of an electron with spin $\sigma$ at $i$th site. The first (second) term describes the hopping of electrons between the nn (nnn) sites $\langle i,j \rangle$ ($\langle\langle i,j \rangle\rangle$) on the square lattice, and the third term represents the on-site Coulomb interactions ($U>0$). In the following, we focus on the half filling, i.e., the filling is given by $n = N_s^{-1} \sum_\sigma \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle = 1$ ($N_s = L \times L$ is the system size). To reduce the numerical cost, we only consider the total $S^z = 0$ space, i.e., $S^{\text{total}} = \sum_i S_i^z = 0$. We employ a $4 \times 4$ cluster with a periodic boundary condition in the most of the present Letter [19].
In the TPQ method \cite{18}, by multiplying \((l - \hat{H}/N_s)\) to random vector \(|\psi_{\text{rand}}\rangle\), we numerically generate the TPQ state. Here, \(l\) is constant that is larger than the maximum eigenvalue of \(\hat{H}/N_s\). The \(k\)th TPQ state is recursively defined as \(|\psi_k\rangle \equiv (l - \hat{H}/N_s)|\psi_{k-1}\rangle/|(l - \hat{H}/N_s)|\psi_{k-1}\rangle\) with \(|\psi_0\rangle = |\psi_{\text{rand}}\rangle\). It is shown that the temperature \(T_k\) corresponding to the \(k\)th TPQ state is estimated from the \(k\)th internal energy \(u_k = \langle \psi_k | \hat{H} | \psi_k \rangle / N_s\) within the accuracy of \(O(1/N_s)\), as \(\beta_k = 1/k_BT_k = 2k/N_s(l - u_k) + O(1/N_s)\), where \(k_B\) is the Boltzmann constant and we take \(k_B = 1\) in this letter. It is shown that physical properties at \(T = T_k\) can be calculated as the expectation value taken with respect to \(|\psi_k\rangle\), i.e., \(\langle A \rangle_{T = T_k} = \langle \psi_k | \hat{A} | \psi_k \rangle / O(1/N_s)\).

To estimate the finite-size error, we typically perform five runs initiated with different \(|\psi_{\text{rand}}\rangle\) and regard its standard deviations as error bars. Here, note that, in the pioneering works \cite{20,22}, the finite-temperature observables were already calculated by replacing ensemble average with random sampling of wave functions.

\textit{Finite-temperature physical quantities in Hubbard models.}—We first show the results of the finite-\(T\) calculations for \(t'/t = 0.5\) as an example of weakly frustrated Hubbard models. The ground state is expected to be Néel state for \(t'/t > 0.5\). Figure 2(a) shows that temperature dependence of the specific heat \(C/N_s\), which is given by \(C/N_s = (\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2) / (N_s T^2)\). The specific heat has a single peak for \(U/t = 4\) as a function of \(T\) while double-peak structures \cite{23} are universal at strong-coupling regions of the Hubbard-type models irrespective of dimensionality [23,27].

The high-temperature peak of \(C\) is generated by the charge degrees of freedom \cite{23,28} whose energy scale is determined by \(U\), as confirmed later by the peak temperatures insensitive to \(t'\) shown in Fig. 4(c). Below the peak temperature, the Mott gap opens and charge degrees of freedom begin to freeze. In other words, below the peak temperature, electrons begin to feel the on-site repulsion \(U\) and double occupancy, which is measured by \(D = N_s^{-1} \sum_{i=1}^{N_s} \langle n_{i\uparrow} n_{i\downarrow}\rangle\), is gradually prohibited. We show temperature dependence of the double occupancy in Fig. 2(b). Our simulation shows non-monotonic temperature dependence of \(D\) from weak to strong coupling region, i.e., \(D\) has the minimum around \(T/t \sim 1\).

We note that this non-monotonic behavior is universal one and observed in a wide range of Hubbard-type models [29,32]. The non-monotonic temperature dependence is explained by the development of antiferromagnetic correlations. Because the antiferromagnetic correlations in...
duce singlet states that have larger double occupancies compared to the other states, the double occupancy increases at low temperature.

The low-temperature peak of the specific heat, in contrast to the high-temperature peak, is induced by spin degrees of freedom [23–27]. This signals development of antiferromagnetic correlations as shown in Fig. 2(c), which corresponds to an increase in \( D \) at low temperatures as discussed above. The peak temperature becomes lower as \( U \) increases, as is manifest in Fig. 2(a), which is consistent with the characteristic energy scale of the spin-degrees of freedom at the strong coupling limit given by the effective superexchange \( J_1 \sim 4t^2/U \). To examine the energy scale, we show the temperature dependence of \( D \) for several temperatures as shown in Fig. 2(c). As it is expected, the spin correlations develop around the low-temperature peak of the specific heat. The two emergent energy scales corresponding to spin and charge degrees of freedom in the strong coupling region are indeed identified as origin of two-peak structure of the specific heat for \( U/t \geq 6 \) while separation of these energy scales may not be clear in excitation spectra [26].

Effect of geometrical frustration on metal-insulator transitions.—To examine the signature of the finite-temperature Mott transitions, we calculate the \( U \)-dependence of \( D \) for several temperatures as shown in Fig. 2(d). By lowering the temperatures, we find the slope of \( D \) becomes steep. Since the slope of \( D \) diverges at the finite-temperature Mott critical end point [52], this behavior can be regarded as the crossover of the finite-temperature Mott critical point.

To see the \( t' \) dependence of the critical temperatures of the Mott transitions from the crossover behaviors at fixed temperature, we calculate the \( U \) dependence of \( D \) for several different \( t' \) at \( T/t = 0.1 \) as shown in Fig. 3(a). From this data, by performing the numerical differentiation for \( D \) with respect to \( U \), we obtain doublon susceptibility \( \chi_D = -\partial D/\partial U \). Here, note that, even at zero temperature, the maxima of \( \chi_D \) as the function of \( U/t \) have been demonstrated to signal the Mott transitions in the finite-size Hubbard models [35]. The obtained \( \chi_D \) is shown in Fig. 3(b). By increasing \( t' \) (increasing frustration), we find that the peak values of \( \chi_D \) at fixed temperature decrease and the peak almost vanishes around \( t'/t \sim 0.75 \). This result indicates that the critical temperature of the critical end point of the Mott transitions becomes lower by increasing the frustration and the marginal quantum critical point (MQCP) [38] exists around \( t'/t \sim 0.75 \), where the critical temperature of the Mott transition becomes zero. Because of the limitation of the available system size, it is hard to make a conclusion to the fate of the finite-temperature Mott critical point. However, our results are qualitatively consistent with the mean-field calculations [37, 38] and it is plausible that the MQCP appears around \( t'/t \sim 0.75 \). We note that ground-state calculations for the Hubbard model on the anisotropic triangular lattice also indicate that nature of Mott transitions is governed by the geometrical frustrations [39].

Signatures of QSL.—Here, to examine the signature of the spin liquid state, we calculate spin correlations for several different \( t' \). As shown in Fig. 4(a) and (b), in the small \( t'/t \) (\( t'/t \leq 0.6 \)), by lowering the temperature, antiferromagnetic nn spin correlations develop while the ferromagnetic nnn spin correlations develop. These spin correlations are consistent with the Néel order. In contrast to this, for large \( t' \) region (\( t'/t \geq 0.8 \)), while the antiferromagnetic nn spin correlations develop, the nn spin correlations remain small even at low temperatures below \( t/10 \). These spin correlations indicate that the stripe antiferromagnetic order becomes stable in the large \( t' \) region. Sandwiched by the Néel and the stripe orders, \( S_{nnn} \) is saturated and remains small even at low temperatures for the intermediate \( t' \). We note that short-range spin correlations at moderately high temperatures (\( T/t \sim 0.1 \)) reflect the corresponding ground states and the behavior at \( t'/t = 0.75 \) is consistent with that of the QSL.

We next examine the thermodynamic properties of the spin-liquid candidates. In contrast to the high-temperature peaks of \( C \) insensitive to \( t' \) shown in Fig. 4(c), the positions of the second peak largely depend on \( t' \) since they are governed by the spin degrees of freedom. At the highly frustrated parameter region \( t'/t \sim 0.75 \), the amplitude of the second peak remains small and indicates the substantial amount of low-energy excitations is left even below the energy scale \( T/t \sim 0.05 \).

To quantify the amount of the low-energy excitations, we calculate the entropy. We show temperature dependence of \( S_{norm} \) in Fig. 4(d). At the highly frustrated region (\( t'/t=0.75 \)), the entropy is not released down to \( T/t \sim 0.05 \) compared to weakly frustrated regions.
The reduction of the low-temperature-peak height occurs at $t'/t = 0.75$ compared to the region where the magnetic long-range orders appear.

We also show $t'$ dependence of the entropy at several fixed temperatures in Fig. 4(f). We find that the entropy at fixed temperature has peak around $t'/t \sim 0.75$, where the spin-liquid or non-magnetic ground states are expected at the strong coupling limit [16, 17]. In sharp contrast, for the Néel and stripe order, the entropy quickly becomes zero by decreasing the temperature, which indicates that almost all the degrees of freedom including spin degrees of freedom is released below $T \sim t/10$.

Even at the moderately high temperatures $T \sim t/10$, therefore, the entropy clearly shows whether the target systems have chance to be spin-liquid states at zero temperature. This fact is seemingly trivial since, in the presence of the geometrical frustrations, entropy is expected to remain finite at low temperatures well below the exchange coupling $J_1$. However, the present result offers the first unbiased and quantitative criterion for the emergence of the spin-liquid ground states in the geometrically frustrated Mott insulators. Although competition among quantum phases is also expected to show remaining entropy, there are counterexamples. An example is the quantum phase transition from the Kitaev spin liquid [10] to ordered states [11]. When the ground state changes from the spin liquid to an ordered state, entropy at a temperature equal to, for example, one-quarter of the dominant energy scale monotonically decreases and does not show any enhancement above the transition point [12].

In summary, we apply the TPQ method to the frustrated Hubbard model. By calculating the susceptibilities of the double occupancy, we find that the characteristic energy scale of the Mott transition becomes lower by increasing $t'$. This result indicates emergence of the MQCP around $t'/t \sim 0.75$. We note that the MQCP and QSL appear around nearly the same parameter region and we expect that this coincide is not accidental: Since infinitesimally small antiferromagnetic order parameters cannot generate a single-particle gap on the entire Fermi surface, another exotic phases such as the quantum phases is also expected to show remaining entropy.

The large remaining entropy is observed at $t'/t \sim 0.75$, the large remaining entropy is observed and it is the evidence of QSL.

To examine the finite-size effects, we show the specific heat of the 18-site cluster compared with that for the larger $U/t$ and the strong coupling limit [19] in Fig. 4(e) by setting $J_1 = 4t^2/U$ and $J_2 = 4t^2/U$, at the highly frustrated parameter $t'/t = 0.75$. Although small system size dependence exists, all the data consistently shows that the low-temperature-peak height occurs at $t'/t = 0.75$ compared to the region where the magnetic long-range orders appear.

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it is an intriguing challenge to examine whether the proposal will work.

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