Quantum Monte Carlo study of the half-filled Hubbard model on the honeycomb lattice

Yuichi Otsuka\textsuperscript{1}, Seiji Yunoki\textsuperscript{1,2,3} and Sandro Sorella\textsuperscript{1,4,5}

\textsuperscript{1}Computational Materials Science Research Team, RIKEN AICS, Kobe, Hyogo 650-0047, Japan,
\textsuperscript{2}Computational Condensed Matter Physics Laboratory, RIKEN ASI, Saitama 351-0198, Japan,
\textsuperscript{3}CREST, Japan Science and Technology, Kawaguchi, Saitama 332-0012, Japan,
\textsuperscript{4}SISSA – International School for Advanced Studies, Via Bonomea 265, 34136 Trieste, Italy, and
\textsuperscript{5}Democritos Simulation Center, CNR – IOM Instituto Officina dei Materiali, 34151 Trieste, Italy

E-mail: otsukay@riken.jp

Abstract. The half-filled Hubbard model on the honeycomb lattice is investigated by numerically exact large-scale quantum Monte Carlo simulations for lattice sizes up to 2592 sites. By performing careful finite-size scaling for the spin-spin correlation functions, calculated with a high degree of accuracy, we find that the ground state is antiferromagnetically long-range ordered at $U/t = 4$, where $U$ is the on-site Hubbard interaction and $t$ is the nearest neighbor hopping. Our result is in sharp contrast to a recent report [Meng et al., Nature 464, 847 (2010)], where instead strong evidence of spin liquid behavior is found.

1. Introduction

The Hubbard model, consisting of the on-site repulsive interaction $U$ and the nearest neighbor hopping $t$, has been extensively investigated as the canonical model for strongly correlated electron systems, especially since the discovery of high-$T_c$ cuprate superconductors [1]. On the square lattice at half filling, the model exhibits the Mott transition from a paramagnetic metal to an antiferromagnetic insulator (AFMI) upon inclusion of an infinitely small repulsive interaction $U$. This is due to the perfect nesting of the non-interacting Fermi surface for the square lattice, as well as a Van Hove singularity characteristic in the density of states [2]. In the case of the honeycomb lattice, there are no such instabilities, though the lattice is still bipartite. Therefore, we expect the Mott transition to occur at a finite value of the interaction, $U_c$. Indeed, the Mott transition from a semi-metal (SM) to the AFMI at $U_c/t \approx 4.5$ was reported two decades ago [3].

Recently, the discovery of graphene [4] has triggered renewed interests in the half-filled Hubbard model on the honeycomb lattice [5]. Among many works, Meng et al. [6] have recently reported that a gapped spin liquid phase without any broken symmetry resides between SM and AFMI. Their finding is rather surprising because it is widely believed that only large quantum fluctuations, usually induced by geometrical frustration, can stabilize a true spin liquid in the ground state. Therefore, the possibility to have a true spin liquid in the simple honeycomb lattice deserves much more careful analysis.
In this paper, using a numerically exact quantum Monte Carlo method at zero temperature, we reexamine the Hubbard model on the honeycomb lattice with much larger clusters containing up to 2592 sites. We perform careful extrapolations of our numerical data to the thermodynamic limit (TDL) in order to estimate an antiferromagnetic (AF) order parameter which should have a strong finite-size effect near the phase boundary. Here, we focus on the case of $U/t = 4$, where the strongest evidence of the spin liquid behavior was previously found [6]. We show numerical evidence that the ground state is instead antiferromagnetically ordered.

2. Model and method

The Hubbard model on the honeycomb lattice is described by following Hamiltonian,

$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow},$$

(1)

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (annihilates) an electron of spin $\sigma(=\uparrow, \downarrow)$ at site $i$, $\langle i,j \rangle$ runs over a pair of nearest neighbor sites $i$ and $j$, and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. We consider finite-size clusters of $N = 2L^2$ sites with $L$ being the linear dimension, as shown in figure 1(a) for $L = 3$. We assume periodic boundary conditions and that $L$ is a multiple of 3, so that the two inequivalent Dirac points $K$ and $K'$ [figure 1(b)], expected to be relevant for low-energy properties, are allowed in momentum space. Therefore, we use $L = 3, 6, 9, 12, 15, 18, 24, \text{ and } 36$.

Since the honeycomb lattice is bipartite and the particle-hole symmetry holds at half filling, the auxiliary fields quantum Monte Carlo method [2] is the most powerful tool to calculate the exact ground state correlation functions of the model (1) for large $L$, without being vexed by the negative sign problem [3]. Here, we employ the ground-state auxiliary field quantum Monte Carlo method to evaluate the ground state expectation value $\langle O \rangle$ of any physical observable $\hat{O}$ by first calculating

$$O(\tau) = \frac{\langle \psi_L | e^{-\frac{\tau}{2} \hat{H}} \hat{O} e^{-\frac{\tau}{2} \hat{H}} | \psi_R \rangle}{\langle \psi_L | e^{-\tau \hat{H}} | \psi_R \rangle}$$

(2)

and then taking the limit $\tau \to \infty$, i.e., $\langle O \rangle = \lim_{\tau \to \infty} O(\tau)$. Here, $\langle \psi_L \rangle$ and $| \psi_R \rangle$ are referred to the left and right trial (initial) wave functions, respectively, both of which are chosen so as not to be orthogonal to the exact ground state wave function. For the former, we take $| \psi_L \rangle = \hat{P}_G | \Phi_{\text{MF}} \rangle$, where $\hat{P}_G = \prod_i \exp (-gn_{i\uparrow} n_{i\downarrow})$ is the partial Gutzwiller projection operator and $| \Phi_{\text{MF}} \rangle$ is the
mean-field solution of (1) with AF order parameter $\Delta$ (ordered along the $x$ direction). For the latter, we use a simple Slater determinant of $N$ electrons, the ground state for $U/t = 0$, with an additional small perturbation term to remove the degeneracy at momenta $K$ and $K'$. It should be noted that these choices are crucial, because they allow fast convergences and stable numerical simulations [7]. The quantum mechanical expression in (2) is mapped onto the (2+1) classical system by means of the Suzuki-Trotter decomposition [8, 9] and by introducing discrete auxiliary fields [2] defined for each time slice and each site. The resulting classical partition function can be evaluated by the standard Monte Carlo method.

Apart for the statistical errors in the sampling, we have three types of systematic errors due to (i) finite projection time $\tau$, (ii) finite width of the Trotter slice $\Delta \tau = \tau/N\tau$ with $N\tau$ being the Trotter number, and (iii) finite system size $L$. All of these should be eliminated by careful extrapolations to accurately estimate the order parameter in the TDL.

3. Results

In order to study the nonmagnetic to AF transition, we calculate the spin structure factor $S_{\text{AF}}/N$ as a function of $\tau t$ (a) and $(\Delta \tau t)^2$ (b) for $U/t = 4$ and different system sizes $L$ indicated in the figures. In (a), the AF order parameter $\Delta$ in $|\psi_L\rangle$ is also indicated. In (b), $\tau t = L + 4$ is fixed and lines are linear fits in $(\Delta \tau t)^2$. The Gutzwiller parameter $g$ in $|\psi_L\rangle$ is 0.71.

![Figure 2. Spin structure factor $S_{\text{AF}}/N$ as a function of $\tau t$ (a) and $(\Delta \tau t)^2$ (b) for $U/t = 4$ and different system sizes $L$ indicated in the figures. In (a), the AF order parameter $\Delta$ in $|\psi_L\rangle$ is also indicated. In (b), $\tau t = L + 4$ is fixed and lines are linear fits in $(\Delta \tau t)^2$. The Gutzwiller parameter $g$ in $|\psi_L\rangle$ is 0.71.](image-url)
of $\tau$ is large enough to obtain converged results in all cases studied. Notice also that the small $\tau$ tends to underestimate the AF order, which implies that our estimate of $m_s$ should be at most a lower bound.

Next, we discuss the effect of the finite width of the Trotter slice $\Delta \tau$. Since we use the symmetric decomposition [8, 9], the systematic error introduced in the expectation value should be $O(\Delta \tau^2)$. Indeed, as shown in figure 2 (b) and figure 3(b), the results for different values of $\Delta \tau$ are well fitted by a linear function of $(\Delta \tau)^2$. By extrapolating to $\Delta \tau \rightarrow 0$, we can in principle eliminate the systematic error due to a finite value of $\Delta \tau$ used in the simulations. However, we find that $\Delta \tau = 0.1$ is already small enough compared to the statistical error. Since among the three types of the systematic errors, only this extrapolation process can result in reducing $m_s$, we analyze the finite size scaling for the results before and after $\Delta \tau \rightarrow 0$.

Finally, we extrapolate $S_{AF}/N$ and $C(L_{max})$ to the TDL by careful finite-size scaling. In figure 4, both $S_{AF}/N$ and $C(L_{max})$ are plotted as a function of $1/L$ [10] and fitted using cubic polynomials. We can see in figure 4 that the consistent AF order parameter $m_s$ is obtained by the finite-size extrapolation of both quantities. This strongly supports that our finite-size extrapolation is reliable. The estimated $m_s^2 = \lim_{L \rightarrow \infty} S_{AF}/N = \lim_{L \rightarrow \infty} C(L_{max})$ is apparently small, which reflects that $U/t = 4$ is very close to $U_c/t$. However, as clearly seen in the inset of figure 4, $m_s^2$ is finite.

To further confirm this result, we summarize in Tables 1 and 2 the results of $m_s^2$ obtained by several fitting procedures using different sets of data for $\Delta \tau t = 0.1, 0.2, 0.4$, and $\Delta \tau t \rightarrow 0$. As shown in Tables 1 and 2, there is a clear tendency that $m_s^2$ is larger when we use the more accurate (namely closer to the TDL) data, which includes the largest size simulations. This tendency is less clear in the results of $C(L_{max})$, but here the finite-size effects are smaller and the statistical errors are much larger compared to those of $S_{AF}/N$. Note, however, that the extrapolated values by $C(L_{max})$ are systematically larger than those of $S_{AF}/N$, which implies that our extrapolated value for $m_s^2$ based on $S_{AF}/N$ can be considered to be a safe lower bound.

We find that the most reliable fit is obtained when we use all data for $L = 6–36$, by judging from the values of the chi-square obtained in the extrapolations. It is also important to note...
that the AF order parameters, estimated for all these different procedures, are finite.

4. Summary

The half-filled Hubbard model on the honeycomb lattice has been investigated by large-scale quantum Monte Carlo simulations. In order to examine whether the antiferromagnetic long-range order exists at $U/t = 4$, we have performed the simulations on lattices containing up to 2592 sites and carefully extrapolated data to the thermodynamic limit. In sharp contrast to the recent report by Meng et al. [6], our results support the existence of the antiferromagnetic long-range order, which suggests that the spin liquid phase is at least reduced to $U/t < 4$ if it ever exists. The results for other $U/t$ and the ground state magnetic phase diagram will be published elsewhere [7].

Table 1. Exaggerated values in the TDL of the spin structure factor, $S_{AF}/N$, (in unit of $10^{-4}$) for $U/t = 4$ and $\Delta \tau = 0.1, 0.2, 0.4$, and $\Delta \tau \rightarrow 0$. The extrapolation is performed using different data sets (indicated in the first column) by cubic polynomials in $1/L$. Chi-square ($\chi^2$) divided by the number of degrees of freedom ($N_{DF}$) is also shown. The numbers of data points used are 6, 7, and 8 for (i)-(iii), (iv) and (v), and (vi), respectively. The statistical errors are indicated by numbers in parentheses (corresponding to the last two digits).

| $L$ | $\Delta \tau = 0.4$ | $\Delta \tau = 0.2$ | $\Delta \tau = 0.1$ | $\Delta \tau \rightarrow 0$ |
|-----|---------------------|---------------------|---------------------|---------------------|
| (i) | 3 - 18              | 8.6(14)             | 1.95                | 3.3(15)             |
| (ii)| 6 - 24              | 13.7(15)            | 1.46                | 8.9(17)             |
| (iii)| 9 - 36             | 16.1(17)            | 0.64                | 6.5(15)             |
| (iv)| 3 - 24              | 10.98(86)           | 2.82                | 5.54(93)            |
| (v) | 6 - 36              | 14.2(11)            | 1.07                | 7.61(83)            |
| (vi)| 3 - 36              | 11.97(64)           | 3.03                | 6.12(53)            |

\[ \chi^2/N_{DF} \]

\[ 1.95, 0.26, 1.61 \]

\[ 2.8(13), 0.45, 5.1(13) \]

\[ 2.44, 0.72, 4.97(74) \]

\[ 2.83, 1.93, 3.78(45) \]
Table 2. Extrapolated values in the TDL of the spin-spin correlation function at the maximum distance, $C(L_{\text{max}})$, (in unit of $10^{-4}$) for $U/t = 4$ and $\Delta \tau t = 0, 0.2, 0.4$, and $\Delta \tau t \rightarrow 0$. The extrapolation is performed using different data sets (indicated in the first column) by cubic polynomials in $1/L$. Chi-square ($\chi^2$) divided by the number of degrees of freedom ($N_{\text{DF}}$) is also shown. The numbers of data points used are 6, 7, and 8 for (i)-(iii), (iv) and (v), and (vi), respectively. The statistical errors are indicated by numbers in parentheses (corresponding to the last two digits).

| $L$ | $\Delta \tau t = 0.4$ | $\Delta \tau t = 0.2$ | $\Delta \tau t = 0.1$ | $\Delta \tau t \rightarrow 0$ |
|-----|----------------|----------------|----------------|----------------|
| (i) | 3 - 18 | 12.2(30) | 4.2(33) | 12.9(37) | 8.9(28) |
| (ii) | 6 - 24 | 14.8(43) | 10.3(40) | 6.6(32) | 8.5(28) |
| (iii) | 9 - 36 | 10.2(38) | 11.5(48) | 10.5(40) | 10.6(36) |
| (iv) | 3 - 24 | 13.0(19) | 7.2(19) | 10.1(19) | 8.8(16) |
| (v) | 6 - 36 | 12.5(25) | 10.7(24) | 8.6(23) | 9.9(20) |
| (vi) | 3 - 36 | 12.4(13) | 8.3(14) | 10.5(15) | 9.5(12) |

Acknowledgments

We acknowledge E. Tosatti, F. Becca, and T. Li for useful discussions. We are also grateful to A. Muramatsu and F. F. Assaad for valuable comments. This work is supported by a PRACE grant 2010PA0447 and by MIUR-COFIN2012. Part of the results is obtained by K computer at RIKEN Advanced Institute for Computational Science.

References

[1] Imada M, Fujimori A and Tokura Y 1998 Rev. Mod. Phys. 70 1039
[2] Hirsch J 1985 Phys. Rev. B 31 4403
[3] Sorella S and Tosatti E 1992 Europhys. Lett. 19 699
[4] Novoselov K S, Geim A K, Morozov S V, Jiang D, Zhang Y, Dubonos S V, Grigorieva I V and Firsov A A 2004 Science 306 666
[5] Neto A H C, Guinea F, Peres N M R, Novoselov K S and Geim A K 2009 Rev. Mod. Phys. 81 109
[6] Meng Z Y, Lang T C, Wessel S, Assaad F F and Muramatsu A 2010 Nature 464 847
[7] Sorella S, Otsuka Y and Yunoki S 2012 Absence of a spin liquid phase in the hubbard model on the honeycomb lattice (Preprint arXiv:1207.1783v1)
[8] Trotter H F 1959 Proc. Amer. Math. Soc. 10 545
[9] Suzuki M 1976 Commun. Math. Phys. 51 183
[10] Reger J D, Riera J A and Young A P 1989 J. Phys.: Cond. Matt. 1 1855