Phase diagram of the magnetic state obtained from a two-particle self-consistent analysis of the half-filled Hubbard model on a honeycomb lattice

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Abstract. Motivated by the fascinating magnetic properties in the half-filled Hubbard model on a honeycomb lattice, we calculate the spin susceptibility and estimate the magnetic transition by applying the two-particle self-consistent (TPSC) method. The diagonalized spin-susceptibility matrix has its maximum at \( Q = 0 \), which indicates that an uniform magnetic order develops between the unit cells. The sign of the spin susceptibility between same sublattices is opposite to that between different sublattices. Therefore, an antiferromagnetic state develops in this system. We calculate the temperature dependence of the Stoner factor and estimate the critical temperature extrapolation. By applying the same analysis to several values of on-site interactions, we present the phase diagram of the magnetic state in the half-filled Hubbard model on a honeycomb lattice. Based on the phase diagram, the critical on-site interaction \( U_c/t \) above which magnetism occurs at the ground state can be estimated as being approximately 3.81.

1. Introduction
Honeycomb lattices have interesting band structures such as a Dirac-like dispersion and the van Hove singularity. The physical properties of this type of lattice have been actively studied, and recently the Kane–Mele model [1] is attracted attentions. For the Hubbard model on a honeycomb lattice with half-filling electrons, the critical on-site interaction \( U_c/t \) above which magnetism occurs at the ground state has been studied [2] and its value has been estimated to be in the range of 3.5–5.0 [3, 4, 5, 6, 7, 8, 9, 10, 11, 12]. The magnetic transition is thought to be caused by antiferromagnetism; however, recent studies suggest the possibility of a spin-liquid state [7]. Recent large-scale quantum Monte Carlo calculations have estimated the critical interaction \( U_c/t \) to be 3.869 ± 0.013 [9] and 3.85 ± 0.02 [12]. The functional renormalization group indicates that \( U_c/t \) is approximately 3.8 [5, 6]. The estimate of the crossover temperature obtained from the two-particle self-consistent (TPSC) method [13] is \( U_c/t = 3.79 ± 0.01 \) [11].

We study the magnetic state in the half-filled Hubbard model on a honeycomb lattice by using the TPSC method. We confirm the wavenumber vector at which the spin susceptibility is maximized and extrapolate the temperature dependence of the Stoner factor that reaches unity at the critical temperature of the magnetic transition. Moreover, we estimate the critical temperature for several on-site interactions and obtain the phase diagram for the magnetic state in the interaction–temperature space. Based on the phase diagram, we estimate the critical on-site interaction \( U_c/t \) at which the magnetic transition occurs at the ground state.
2. Method

We focus on the two-site Hubbard Hamiltonian $H$ given as follows:

$$H = \sum_{\langle i:j \rangle, \sigma} \left\{ t_{i:j} \sigma c_{i \alpha}^\dagger c_{j \beta} + H.c. \right\} + \sum_{i \alpha} U n_{i \alpha} n^\dagger_{i \alpha}, \quad (1)$$

where $i$ and $j$ are the unit cell indices, $\alpha$ and $\beta$ specify the sites in a unit cell, $c_{i \alpha}^\dagger$ ($c_{i \alpha}$) is the creation (annihilation) operator for spin $\sigma$ at site $i$ in unit cell $\alpha$, $t_{i:j}$ is the electronic transfer energy between site $(i, \alpha)$ and site $(j, \beta)$, and $\langle i:j \rangle$ represents the summation of the nearest-neighboring sites. The transfer energy is taken to be $t$ between the nearest-neighboring sites on the honeycomb lattice, as shown in Fig. 1(a). $U$ is the on-site interaction and $n_{i \alpha}$ is the number operator of electrons for spin $\alpha$ at site in the unit cell $i$. By diagonalizing the first term in Eq. (1), we obtain the noninteracting electronic band structure $\xi(k)/t$, as shown in Fig. 1(b). The Dirac points are located at $\xi(k)/t = 0$ on the K point of the Brillouin zone. The density of states (DOS) is represented in Fig. 1(c). The DOS decreases continuously toward $\xi(k)/t = 0$ because the band structure is the linear dispersion around the Dirac points. Conversely, the van Hove singularities at the energy $\xi(k)/t = \pm 1$ on the M point bring about the divergence in the DOS. We set one electron per site, where the band structure is half-filled and the Fermi level coincides with the Dirac point.

![Figure 1](image_url)

Figure 1. (a) Hubbard model on a honeycomb lattice, where the solid and open circles represent the A and B sublattices; the blue dashed rhombus indicates the unit cell, and the red up (down) arrow schematically indicates the up (down) spin of the electron. (b) The electronic band structure along the symmetric $k$-points, where the inset shows the Brillouin zone; and (c) the DOS in the honeycomb lattice.

To consider the effect of electron correlation, we obtained the bare susceptibility and the bare Green function in the site representation given by

$$\chi^0_{\alpha \beta}(q) = -\frac{T}{N_c} \sum_k G^0_{\alpha \beta}(k + q) G^0_{\beta \alpha}(k), \quad (2)$$

$$G^0_{\alpha \beta}(k) = \sum_\gamma d_{\alpha \gamma}(k) d^*_{\beta \gamma}(k) G^0_{\gamma}(k), \quad (3)$$
where $T$ and $N_c$ are the temperature and total number of unit cells, respectively, and $d_{\alpha\gamma}(k)$ is the unitary matrix. The bare Green function in the band representation, $G_0^0(k)$, is given by

$$
G_0^0(k) = \frac{1}{\varepsilon_n - \xi(k)}. \tag{4}
$$

Here we introduce the abbreviations $k = (k, \varepsilon_n)$ and $q = (q, \omega_m)$ for the fermionic and bosonic Matsubara frequencies, respectively. The indices $\alpha\beta$ refer to an element ($\alpha \beta$) of the matrices such as $\hat{\chi}^0(q)$.

The TPSC method has been applied to single-site systems [13, 14], multi-site systems [11, 15, 16, 17], and multi-orbital systems [18]. Within the TPSC scheme, using the bare susceptibility given by Eq. (2), the spin and charge susceptibilities are as follows:

$$
\hat{\chi}^{\text{sp}}(q) = \left( \hat{I} - \hat{\chi}^0(q) \hat{U}^{\text{sp}} \right)^{-1} \hat{\chi}^0(q), \tag{5}
$$

$$
\hat{\chi}^{\text{ch}}(q) = \left( \hat{I} + \hat{\chi}^0(q) \hat{U}^{\text{ch}} \right)^{-1} \hat{\chi}^0(q), \tag{6}
$$

where $\hat{U}^{\text{sp}}$ ($\hat{U}^{\text{ch}}$) is the local spin (charge) vertex, and $\hat{I}$ is the unit matrix. The local vertices are determined by satisfying two sum rules for the local moment:

$$
\frac{2T}{N_c} \sum_q \chi^{\text{sp}}_{\alpha\alpha}(q) = n_\alpha - 2 \langle n_\alpha^\uparrow n_\alpha^\downarrow \rangle, \tag{7}
$$

$$
\frac{2T}{N_c} \sum_q \chi^{\text{ch}}_{\alpha\alpha}(q) = n_\alpha + 2 \langle n_\alpha^\uparrow n_\alpha^\downarrow \rangle - n_\alpha^2, \tag{8}
$$

where $n_\alpha$ is the particle number at site $\alpha$. Here we used the relations $n_\alpha^\uparrow = n_\alpha^\downarrow = n/2$ and $n_{\alpha\sigma} = n_{\alpha\sigma}^2$ from the Pauli principle.

The local spin vertex $\hat{U}^{\text{sp}}$ is related to the double occupancy $\langle n_\alpha^\uparrow n_\alpha^\downarrow \rangle$ by the ansatz

$$
U^{\text{sp}}_{\alpha\alpha} = \frac{\langle n_\alpha^\uparrow n_\alpha^\downarrow \rangle}{\langle n_\alpha^\uparrow \rangle \langle n_\alpha^\downarrow \rangle} U_{\alpha\alpha}, \tag{9}
$$

where $U_{\alpha\alpha}$ is element ($\alpha \alpha$) of the on-site interaction matrix $\hat{U}$. The double occupancy $D_\alpha = \langle n_\alpha^\uparrow n_\alpha^\downarrow \rangle$ is given by

$$
D_\alpha = \frac{U^{\text{sp}}_{\alpha\alpha} n_\alpha^2}{4}. \tag{10}
$$

Equations (5)–(10) give the set of self-consistent equations for the TPSC scheme.

In this study, we show the spin susceptibility obtained from the larger eigenvalue of the matrix to find the dominant magnetic order between the unit cells. In this calculation, we take the system size to be $96 \times 96$ $k$ meshes and 16384 Matsubara frequencies.

### 3. Results

Figure 2(a) [2(b)] shows the maximum (minimum) value of the diagonalized spin-susceptibility matrix for the on-site interaction $U/t = 3.82$ and temperature $T/t = 0.02$, respectively. We find that a uniform magnetic order between the unit cells develops because the spin susceptibility has its maximum at the wavenumber vector $Q = 0$. The site-represented spin susceptibilities, which correspond to the elements of its matrix, are shown in Figs. 2(c) and 2(d). It is favorable
Figure 2. The (a) maximum and (b) minimum values of the diagonalized spin-susceptibility matrix. The site-represented spin susceptibility for (c) same sublattices and (d) different sublattices.

when the spin direction is parallel (opposite) between same (different) sublattices. Therefore, we confirmed that an antiferromagnetic order develops in this system.

In this paper, we regard the diagonalized $\chi^0(Q)\hat{U}_{sp}$ matrix as the Stoner factor and abbreviate it as $U_{sp}\chi_0$, where the wavenumber $Q$ gives the maximum value of the spin susceptibility and $Q = 0$ from Fig. 2. The TPSC method satisfies the Mermin–Wagner theorem in two-dimensional system [13]; therefore, the true magnetic order does not occur in the presented model. In a previous study of the TPSC scheme in the Hubbard model on a honeycomb lattice, the critical temperature was estimated via the crossover temperature obtained from the magnetic correlation length [11]. In our study, we regard the temperature at which the line extrapolating the temperature dependence of the Stoner factor from the high temperature reaches unity as the critical magnetic temperature. In a previous study, we have shown that the estimate of the model reproduced by the first-principles band calculation for a $\beta$-type organic conductor is consistent with experimental results, i.e., the magnetic transition occurs at low temperature [16].

Figure 3(a) represents the Stoner factor $U_{sp}\chi_0$ as a function of the temperature for several on-site interactions $U/t$ in the half-filled system. We can fit the temperature dependence of the Stoner factor with the extrapolating line shown in Fig. 3(a). The critical temperatures for each on-site interaction can be estimated. At the ground state, the extrapolating line below $U/t = 3.8$ cannot reach unity, that is, the magnetic transition appears to be absent below that interaction. The phase diagram in the $U/t-T/t$ space is shown in Fig. 3(b). Based on the interaction dependence of the critical temperature, we find that the estimate of the critical on-site interaction, $U_{c}/t$, is near 3.81, which is consistent with several previous studies [3, 4, 5, 6, 7, 8, 9, 10, 11, 12].
4. Conclusions
We performed a TPSC analysis for the magnetic properties in the half-filled Hubbard model on a honeycomb lattice. The spin-susceptibility matrix indicates that an antiferromagnetic order develops in this system. We evaluated the temperature dependence of the Stoner factor and estimated the critical temperature by extrapolating this factor for the several on-site interactions. Plotting the critical temperature as a function of the on-site interaction, we presented the phase diagram of the magnetic state in the half-filled Hubbard model on a honeycomb lattice. From the phase diagram, we estimated the critical on-site interaction to be $U_c/t \approx 3.81$.

Acknowledgments
This work was supported by JSPS KAKENHI Grant No. 16K17754.

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