Effect of exchange interaction on electronic instabilities in the honeycomb lattice: A functional renormalization group study

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The impact of local and non-local density-density interactions on the electronic instabilities in the honeycomb lattice is widely investigated. Some of early studies proposed the emergence of interaction-induced topologically non-trivial phases, but recently it is denied in several works including renormalization group calculations with refined momentum resolution. We use the truncated unitary functional renormalization group to study the many-body instabilities of electrons on the half-filled honeycomb lattice focusing on effect of the exchange interaction. We show that varying the next-nearest-neighbor repulsion and nearest-neighbor exchange integral can lead to diverse ordered phases, namely, the quantum spin Hall, the spin-Kekulé and some spin- and charge-density-wave phases. The quantum spin Hall phase can be induced by a combination of the ferromagnetic exchange and pair hopping interactions. Another exotic phase, the spin-Kekulé phase develops in a very small region of the parameter space considered. We encounter three-sublattice charge-density-wave phase in a large part of the parameter space. It is replaced by the incommensurate charge density wave when increasing the exchange integral. In order to reduce the computational effort, we derive the explicit symmetry relations for the bosonic propagators of the effective interaction and propose a linear-response based approach for identifying the form factor of order parameter. Their efficiencies are confirmed by numerical calculations in our work.

I. INTRODUCTION

The experimental realization of graphene has stimulated intensive research activities on this material. Its lattice structure, the two-dimensional honeycomb lattice has been serving as a platform for basic research on exotic many-body phenomena. Considerable effort has been invested into numerical studies on the possible ground states of extended Hubbard models on the honeycomb lattice. Many of these works have explored a variety of possible orderings in the ground states of the systems with different interaction strengths.

Raghu et al. suggested that a topologically non-trivial quantum anomalous Hall (QAH) state could be emerged on the honeycomb lattice from a large next-nearest-neighbor repulsion $V_2$ since an effective spin-orbit interaction is generated by mean-field decoupling of this term. Further mean-field studies also showed evidence of the existence of the interaction-driven QAH state of spinless fermions on the honeycomb lattice. Another type of topologically non-trivial phases emerged by only a nearest-neighbor interaction $V_1$ has been reported away from half-filling.

The poorly screened Coulomb interaction in the system at half-filling may also develop another conventional orders, such as bond order, charge order, and magnetic order, which then compete with the QAH. For the spinless Hubbard model which has Coulomb interactions between nearest-neighbor sites ($V_1$) and between next-nearest-neighbor sites ($V_2$), mean-field calculations proposed the existence of a Kekulé bond order phase. This phase has also been reported in Refs. 8–10. Exact diagonalization (ED), infinite density matrix renormalization group (iDMRG) studies have considered the stability of the QAH ground state and found various charge-density-wave (CDW) states competing with QAH.

For the spinful Hubbard model an on-site repulsion $U > 0$ between electrons with opposite spins is added, which generates the intricate interplay between charge and spin degrees of freedom. The dominant on-site Coulomb repulsion favors an antiferromagnetic spin-density-wave (SDW) phase. The combination of on-site $U$, nearest-neighbor $V_1$ and next-nearest-neighbor $V_2$ repulsions introduces the possibility of a spinful version of QAH, i.e., the quantum spin Hall (QSH) state, and it is expected that there is more complicated competition or coexistence of different ordering tendencies including the conventional CDW, SDW and QSH.

A number of recent studies of the extended Hubbard model on the honeycomb lattice by means of ED, iDMRG, quantum Monte Carlo (QMC), and functional renormalization group (FRG) indicate a suppression of the QSH or QAH by conventional ordered phases, mainly CDW, at half-filling. This discrepancy on existence of the topologically non-trivial phases needs more research on possible ground states of the honeycomb lattice by more effective and credible approaches. On the other hand, many of these works have considered only the correlation effects by the Coulomb repulsion between electrons, e.g., the parameters $V_1$ and $V_2$. It is natural to expect that the inclusion of the exchange interaction between nearest-neighbor sites would give even richer ground-state phase diagram for the honeycomb lattice at half-filling.

In this work, we investigate the quantum many-body instabilities of electrons on the half-filled honeycomb lattice focusing on the effect of the nearest-neighbor exchange interaction $J$. The effect of the nearest-neighbor
repulsion $V_1$ is relatively well-understood. Beyond a critical coupling strength, $V_1$ destabilizes the semi-metallic phase and the system undergoes a direct and continuous quantum phase transition to a fully gapped CDW phase with opposite charge configuration on two sublattices. While the effect of parameter $V_1$ on ground state of half-filled honeycomb lattice was investigated in many preceding studies, the effect of $V_2$ and $J$ on it appears to be far from clear. Therefore we use the extended Hubbard model with on-site repulsion $U$, next-nearest-neighbor repulsion $V_2$, and nearest-neighbor exchange interaction $J$ for interacting electrons on the honeycomb lattice. 

The main goal of this work is to explore the existence of QSH and the effect of the exchange interaction on the electronic instabilities. To this end, we employ the recently developed truncated unity functional renormalization group (TUFRG) approach for correlated fermions with high resolution of wave-vector dependences in the effective interaction. In addition, we present the symmetry relations for the bosonic propagators which can reduce 1/12 times the computational effort in the case of honeycomb lattice. We also propose an efficient approach to estimate the form factor of factor parameter from the TUFRG results of the effective interaction, which is based on the analysis of the linear response of the system to virtual infinitesimal external fields coupled to the fermion bilinears.

The paper is organized as follows. In Sec. II we introduce Hamiltonian of the extended Hubbard model for spin-1/2 fermions on the honeycomb lattice and TUFRG approach. In Sec. III we derive symmetry relations for the effective interactions and bosonic propagators of electrons in the system, and discuss method to estimate the form factors of various order parameters in three channels, i.e., the pairing, spin and charge channels. In Sec. IV we present and analyze a tentative phase diagram for electrons subjected to on-site, next-nearest-neighbor repulsions and nearest-neighbor exchange interaction. Finally, in Sec. V we draw our conclusions.

II. MODEL AND METHOD

A. Extended Hubbard model

We study spin-1/2 fermions on the honeycomb lattice at half-filling which interact with each other via on-site repulsion $U$, next-nearest-neighbor repulsion $V_2$, and nearest-neighbor exchange interaction $J$. For simplicity, we neglect the nearest-neighbor repulsion $V_1$. The Hamiltonian of the extended Hubbard model is composed of a single-particle part $H_0$ and an interaction part $H_{\text{int}}$:

$$H = H_0 + H_{\text{int}},$$

where $H_0$ is described by a tight-binding Hamiltonian with nearest-neighbor hopping $t$ for honeycomb lattice at half-filling (i.e. $\mu = 0$)

$$H_0 = -t \sum_{\langle i,j \rangle, \sigma} (c_{i,A,\sigma}^\dagger c_{j,B,\sigma} + h.c.).$$

Here the operator $c_{i,o,\sigma}^\dagger$ ($c_{i,o,\sigma}$) creates (annihilates) an electron at lattice site $i$ in the sublattice (orbital) $o$ with spin polarity $\sigma$. The unit of length is set to lattice constant, $a$, i.e., the distance between next-nearest-neighbor sites. The interaction part of the Hamiltonian is given by

$$H_{\text{int}} = U \sum_{i,o} n_{i,o,\uparrow} n_{i,o,\downarrow} + V_2 \sum_{i,o,o',\sigma,\sigma'} n_{i,o,\sigma} n_{i,o',\sigma'}/(i,o,j) + o,\sigma,\sigma'$$

$$+ J \sum_{\langle i,A,j,B \rangle, \sigma,\sigma'} c_{i,A,\sigma}^\dagger c_{j,B,\sigma'} c_{i,A,\sigma'}^\dagger c_{j,B,\sigma} + h.c.),$$

where $n_{i,o,\sigma} = c_{i,o,\sigma}^\dagger c_{i,o,\sigma}$ is the local electron density operator and the sums $\sum_{\langle i,A,j,B \rangle}$ and $\sum_{\langle i,o,j \rangle}$ run over nearest and next-nearest neighbors, respectively. The terms in Eq. (3) describe the on-site Coulomb interaction, next-nearest-neighbor Coulomb interaction, the nearest-neighbor ferromagnetic exchange, and nearest-neighbor pair hopping. (For the real $p_z$ orbitals, the ferromagnetic exchange is accompanied by the pair hopping as in Eq. (3).) Although the magnitude of $J$ is known to be rather small in realistic systems, we artificially enhance it to investigate its effect on the ground state using TUFRG.

B. Truncated unity functional renormalization group method

The TUFRG method is a modification of the functional renormalization group (FRG) method which has been applied to a large number of two-dimensional lattice systems, e.g., the honeycomb lattice, cuprates, and pnictides. It is based on prior channel-decomposed FRG and singular-mode FRG (SMFRG) schemes. The advantage of the TUFRG is the increased momentum resolution in the low-energy effective interaction achieved by numerically efficient scheme. We use the orbital picture of TUFRG which ensures excellent convergence in the expansion of the effective interaction. The $\Omega$ scheme is employed as the regulator for infrared divergences. In this scheme the bare propagator $G_{o_1,o_2}^0(\omega, k)$ for Matsubara frequency $\omega$, wavevector $k$ and orbital indices $o_1, o_2$ (for the honeycomb lattice, the orbital index means the sublattices $A$ or $B$) gets modified with energy scale $\Omega$, i.e.,

$$G_{o_1,o_2}^0(\omega, k) \rightarrow G_{o_1,o_2}^0(\omega, k) = \frac{\omega^2}{\omega^2 + \Omega^2} G_{o_1,o_2}^0(\omega, k).$$
The modified propagator $G^0\Omega$ is then used to set up the expression for the generating functional of 1PI vertex functions, which is now scale dependent as well, $\Gamma \rightarrow \Gamma^\Omega$. The functional flow equation is generated by differentiating $\Gamma^\Omega$ with respect to $\Omega$, which produces a hierarchy of flow equations for the vertex functions. For our analysis we use a truncation in which all $n$-particle vertices with $n \geq 3$ and self-energy feedback are neglected. Such approximation has been proved to be suitable in weak-coupling regimes\textsuperscript{22}. For the spin-SU(2) invariant systems, two-particle part of the generating functional is expressed in terms of the two-particle vertex functions (i.e. the effective interactions) $V^{\Omega}$ and the Grassmann variables $\bar{\psi}, \psi$ as follows:

$$\Gamma^\Omega(\bar{\psi}, \psi) = \frac{1}{2} \int d\xi_1 \cdots d\xi_4 \, V^\Omega_{\alpha_1 \alpha_2, \alpha_3 \alpha_4}(k_1, k_2; k_3, k_4) \delta(k_1 + k_2 - k_3 - k_4) \sum_{\sigma, \sigma'} \bar{\psi}_\sigma(\xi_1) \bar{\psi}'_{\sigma'}(\xi_2) \psi_{\sigma'}(\xi_3) \psi_\sigma(\xi_4),$$

where $k_i = (\omega_i, k_i)$ and $\xi_i = (\omega_i, k_i, \alpha_i)$ are multi-indices gathering a Matsubara frequency $\omega_i$, wavevector $k_i$ and orbital index $\alpha_i$, and $\int d\xi_i$ stands for the notation $\int \frac{d\xi_i}{S_{BZ}} \sum_{\omega_i, \alpha_i}$, with Brillouin zone area $S_{BZ}$ and inverse temperature $\beta$. Since the most singular part of the effective interaction comes from the zero frequency and we are interested in ground-state properties, we will neglect the frequency dependence of it, with external frequencies set to zero. Then the flow equation for the interaction consists of three contributions\textsuperscript{22}

$$\frac{d}{d\Omega} V^{\Omega}_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2}(k'_1, k'_2; k_1, k_2) = J^{pp}_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2}(k'_1, k'_2; k_1, k_2) + J^{ph,cr}_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2}(k'_1, k'_2; k_1, k_2) + J^{ph,d}_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2}(k'_1, k'_2; k_1, k_2), \quad (4)$$

where the particle-particle, crossed and direct particle-hole contributions read

$$J^{pp}_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2}(k'_1, k'_2; k_1, k_2) = - \sum_{\mu, \mu'} \int dp \frac{d}{d\Omega}[G^0\Omega(\omega, p + k'_1 + k'_2)G^{0\Omega}(\omega, \omega - p)] \times V^\Omega_{\alpha'_1 \alpha'_2, \mu \mu'}(k'_1, k'_2; p + k'_1 + k'_2) \cdot V^\Omega_{\alpha_1 \alpha_2, \mu \mu'}(p + k'_1 + k'_2, p; k_1, k_2),$$

$$J^{ph,cr}_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2}(k'_1, k'_2; k_1, k_2) = - \sum_{\mu, \mu'} \int dp \frac{d}{d\Omega}[G^0\Omega(\omega, p + k'_1 - k'_2)G^{0\Omega}(\omega, \omega - p)] \times V^\Omega_{\alpha'_1 \alpha'_2, \mu \mu_0}(k'_1, k'_2; p + k'_1 - k'_2) \cdot V^\Omega_{\alpha_1 \alpha_2, \mu_0 \mu_0'}(p + k'_1 - k'_2, p; k_1, k_2),$$

$$J^{ph,d}_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2}(k'_1, k'_2; k_1, k_2) = - \sum_{\mu, \mu'} \int dp \frac{d}{d\Omega}[G^0\Omega(\omega, p + k'_1 - k'_2)] \times V^\Omega_{\alpha'_1 \alpha'_2, \mu \mu_0}(k'_1, k'_2; p + k'_1 - k'_2) \cdot V^\Omega_{\mu_0 \mu_0', \alpha_1 \alpha_2}(p + k'_1 - k'_2, p; k_1, k_2) + V^\Omega_{\alpha'_1 \alpha'_2, \mu \mu_0}(k'_1, k'_2; p + k'_1 - k'_2) \cdot V^\Omega_{\mu_0 \mu_0', \alpha_1 \alpha_2}(p + k'_1 - k'_2, p; k_1, k_2) - 2V^\Omega_{\alpha'_1 \alpha'_2, \mu \mu_0}(k'_1, k'_2; p; k_1 + k_2),$$

with shorthand notation $\int dp = \int \frac{d\xi_i}{S_{BZ}} \sum_{\omega_i}$ and implicit constraint $k'_1 + k'_2 = k_1 + k_2$. Below we explain a main algorithm of the TUFGRF pointing out a little difference to Ref.\textsuperscript{14}.

The effective interactions can be expressed by a decomposition into single-channel coupling functions

$$V^{\Omega}_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2}(k'_1, k'_2; k_1, k_2) = V^{(0)}_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2}(k'_1, k'_2; k_1, k_2) + \phi^{SC}_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2}(k'_1 + k'_2; -k'_2, -k_2)$$

$$+ \phi^{D}_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2}(k'_1 - k_2; k_2, k'_2) + \phi^{D}_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2}(k'_1 - k_1; k_1, k'_2), \quad (6)$$

where $V^{(0)}$ is the initial bare interaction and is obtained by the Fourier transform of the interaction Hamiltonian in Eq.\textsuperscript{3}. The Eq. (6) has no momentum like $(k_1 - k_2)/2$ in Eq. (5) of Ref.\textsuperscript{14}, which ensures the periodicity of the reciprocal lattice for the $\Phi$ functions. The coupling functions $\Phi$ are developed during the flow according to

$$\frac{d}{d\Omega} \phi^{SC}_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2}(k'_1 + k'_2; -k'_2, -k_2) = J^{pp}_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2}(k'_1, k'_2; k_1, k_2),$$

$$\frac{d}{d\Omega} \phi^{C}_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2}(k'_1 - k_2; k_2, k'_2) = J^{ph,cr}_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2}(k'_1, k'_2; k_1, k_2),$$

$$\frac{d}{d\Omega} \phi^{D}_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2}(k'_1 - k_1; k_1, k'_2) = J^{ph,d}_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2}(k'_1, k'_2; k_1, k_2). \quad (7)$$
Taking into account the strong dependence on transfer momenta (first argument) and weak dependence on other momenta, one can expand the coupling functions \( \Phi \) in a suitable scale-independent basis \( f_m \) and three bosonic propagators \( P, C, D \)

\[
\Phi_{\phi_{ij}, \sigma_{12}}^{SC}(q; p, k) = \sum_{m, n} P_{\phi_{ij}, \sigma_{12}m, \sigma_{12}n}(q) f_m(p) f_n(k),
\]

\[
\Phi_{\phi_{ij}, \sigma_{12}}^{C}(q; p, k) = \sum_{m, n} C_{\phi_{ij}, \sigma_{12}m, \sigma_{12}n}(q) f_m(p) f_n(k), \quad \Phi_{\phi_{ij}, \sigma_{12}}^{D}(q; p, k) = \sum_{m, n} D_{\phi_{ij}, \sigma_{12}m, \sigma_{12}n}(q) f_m(p) f_n(k).
\]

(8)

Note that the \( P, C, D \) matrices have different sequences of the orbital indices in Eq. (8). In practical computation the infinite basis has to be truncated and the truncation error is generally smaller for the orbital picture than one for the band picture. Then the coupling functions are represented by three matrices \( P, C \) and \( D \), each having just one momentum dependence. It enables us to perform calculation with high momentum resolution. Combination of Eqs. (5)–(8) yields the flow equation for the bosonic propagators containing intricate terms in which internal bosonic propagators appear in the fermionic loops and have to be integrated out giving challenge in calculation. With insertions of truncated partitions of unity the fermionic propagators are decoupled from the bosonic propagators yielding very simplified flow equation. The ultimate flow equation for the bosonic propagators reads

\[
\frac{dP}{dt}(q) = V^P(q) \chi_{PP}(q) P(q),\quad \frac{dC}{dt}(q) = V^C(q) \chi_{ph}(q) C(q),
\]

\[
\frac{dD}{dt}(q) = [V^C(q) - V^D(q)] \chi_{ph}(q) V^D(q) + V^D(q) \chi_{ph}(q) [V^C(q) - V^D(q)],
\]

(9)

where

\[
\chi_{PP}^{\phi_{ij}, \sigma_{12}m, \sigma_{12}n}(q) = -\int d\omega \left( C_{\phi_{ij}, \omega, \sigma_1, \omega, \sigma_2} G_{\phi_{ij}, \sigma_1, \sigma_2}^0(\omega, k + q + \mathbf{q}, -\omega, -k) f_m(k) f^*_n(k),
\]

\[
\chi_{ph}^{\phi_{ij}, \sigma_{12}m, \sigma_{12}n}(q) = -\int d\omega \left( C_{\phi_{ij}, \omega, \sigma_1, \omega, \sigma_2} G_{\phi_{ij}, \sigma_1, \sigma_2}^0(\omega, k + q + \mathbf{q}, -\omega, -k) f_m(k) f^*_n(k),
\]

(10)

and \( V^P,C,D \) are projections of the effective interactions onto the form of the three channels,

\[
V^P_{\phi_{ij}, \sigma_{12}m, \sigma_{12}n}(q) = \frac{1}{2} \int_{SBZ} dp \int dp' f_m(p) f^*_m(p') V^P_{\phi_{ij}, \sigma_{12}m, \sigma_{12}n}(p + q, -p; p + q, -p'),
\]

\[
V^C_{\phi_{ij}, \sigma_{12}m, \sigma_{12}n}(q) = \frac{1}{2} \int_{SBZ} dp \int dp' f_m(p) f^*_m(p') V^C_{\phi_{ij}, \sigma_{12}m, \sigma_{12}n}(p + q, -p; p + q, -p'),
\]

\[
V^D_{\phi_{ij}, \sigma_{12}m, \sigma_{12}n}(q) = \frac{1}{2} \int_{SBZ} dp \int dp' f_m(p) f^*_m(p') V^D_{\phi_{ij}, \sigma_{12}m, \sigma_{12}n}(p + q, -p; p + q, -p').
\]

(11)

The bare propagator \( G^0_{\alpha\beta}(\omega, k) \) in the orbital picture is

\[
G^0_{\alpha\beta}(\omega, k) = \sum_b T_{ob}(k) T^*_{ob}(k) (i\omega - E_b(k))^{-1}.
\]

Here \( E_b(k) \) is the one-particle energy of the electron with the wavevector \( k \) in the band \( b \) and \( T_{ob}(k) \) is the element of the transformation matrix between the annihilation operators in orbital picture, \( c_{k,\alpha,\sigma} \), and ones in band picture, \( b_{k,\beta,\sigma} \), namely, \( c_{k,\alpha,\sigma} = \sum_b T_{ob}(k) b_{k,\beta,\sigma} \). By substituting Eqs. (6) and (8) into Eq. (11), one can represent the projections of the effective interactions of Eq. (11) in terms of three matrices \( P, C \) and \( D \) thus obtaining expression of the flow equation (9) via only these matrices. When we choose the plane wave, \( f_m(p) = e^{iR_m \cdot p} \), as basis, the Eq. (11) gives

\[
V^P(q) = V^{P,(0)}(q) + P(q) + V^{P,(C)}(q) + V^{P,(D)}(q),
\]

\[
V^{P,(C)}_{\phi_{ij}, \sigma_{12}m, \sigma_{12}n}(q) = \sum_l \tilde{C}_{\phi_{ij}, \sigma_{12}m, \sigma_{12}n}(R_l; \sigma_1, \sigma_2, R_m + R_n - R_l) e^{i(R_n - R_l) \cdot q},
\]

\[
V^{P,(D)}_{\phi_{ij}, \sigma_{12}m, \sigma_{12}n}(q) = \sum_l \tilde{D}_{\phi_{ij}, \sigma_{12}m, \sigma_{12}n}(R_l; \sigma_1, \sigma_2, R_m + R_n - R_l) e^{-i(R_n - R_l) \cdot q},
\]

\[
V^C(q) = V^{C,(0)}(q) + C(q) + V^{C,(P)}(q) + V^{C,(D)}(q),
\]

\[
V^{C,(P)}_{\phi_{ij}, \sigma_{12}m, \sigma_{12}n}(q) = \sum_l \tilde{P}_{\phi_{ij}, \sigma_{12}m, \sigma_{12}n}(R_l; \sigma_1, \sigma_2, R_m + R_n - R_l) e^{i(R_n - R_l) \cdot q},
\]

\[
V^{C,(D)}_{\phi_{ij}, \sigma_{12}m, \sigma_{12}n}(q) = \sum_l \tilde{D}_{\phi_{ij}, \sigma_{12}m, \sigma_{12}n}(R_l; \sigma_1, \sigma_2, R_m + R_n - R_l) e^{-i(R_n - R_l) \cdot q},
\]

(13)

(14)
\[
V^D(q) = V^{D,(0)}(q) + D(q) + V^{D,(P)}(q) + V^{D,(C)}(q),
\]
\[
V^{D,(P)}_{\alpha'_1\alpha_m\alpha'_2\alpha'_n}(q) = \sum_l \tilde{P}_{\alpha'_1\alpha'_2}(R_l) \hat{r}_{i_1} \cdot \hat{r}_{i_2} R_l - R_{m} - R_{n} (-R_{m}) \cdot q,
\]
\[
V^{D,(C)}_{\alpha'_1\alpha_m\alpha'_2\alpha'_n}(q) = \sum_l \tilde{C}_{\alpha'_1\alpha_2}(R_l) \hat{r}_{i_1} \cdot \hat{r}_{i_2} R_l + R_{m} (-R_{m}) \cdot q,
\]

where \( \tilde{P}(R_m), \tilde{C}(R_m), \tilde{D}(R_m) \) are the Fourier transform of the matrices \( P(q), C(q), D(q) \). In Eqs. (13)–(15), \( V^{P,(0)}(q), V^{C,(0)}(q), \) and \( V^{D,(0)}(q) \), which are obtained by replacing \( V^D \) with \( V^{(0)} \) in Eq. (11), are the projections of the initial effective interactions \( V^{(0)}_{\alpha'_1\alpha_1\alpha'_2}(k_1',k_2';k_1,k_2) \) (i.e. the Fourier transform of the interaction Hamiltonian in Eq. (3)) onto the three channels.

III. SYMMETRIES AND ORDER PARAMETERS

A. Symmetries of bosonic propagators

The structure of the honeycomb lattice is shown in Fig. (1a). The lattice has the \( C_{6v} \) symmetry with respect to the center of hexagons. This symmetry yields the symmetry relations between the bosonic propagators with different momentum transfer. By these relations, the bosonic propagators with transfer momenta in the whole Brillouin zone (BZ) can be generated from ones with transfer momenta in the irreducible region of BZ (see Fig. (1b)), thus reducing the computational effort to 1/12. The symmetry relations are rather complicated in the orbital picture, but when using the plane-wave basis, we can find the explicit symmetry relations for the bosonic propagators. For the expansion of the coupling functions in Eq. (5), we use 13 plane-wave bases with Bravais lattice vectors \( R_m \) shown in Fig. (1c), which are sufficient in the orbital picture.

The Bloch sum of orbitals \( o \) is expressed as

\[
\Psi_{k,o}(r) = \sum_i \Phi_{i,o}(r) e^{i k \cdot R_i} / \sqrt{N},
\]

\[
= \sum_i \Phi_{i}(r - R_i - d_o) e^{i k \cdot R_i} / \sqrt{N},
\]

where \( \Phi_{i}, R_i, d_o \) are the \( \pi \)-orbital wave function, the Bravais lattice vector of the unit cell \( i \) and relative position of the sublattice \( o \), respectively. Under a symmetry operation \( \hat{G} = (Q|t) \) which is a rotation \( Q \) followed by shift \( t \), the function \( \Psi_{k,o}(r) \) is transformed to

\[
\hat{G}\Psi_{k,o}(r) = \exp(-i Q \cdot u_o) \Psi_{Qk,\delta}(r).
\]

Here the Bravais lattice vector \( u_o \) and the orbital index \( \delta \) are determined by

\[
Q d_o + t = u_o + d_\delta,
\]

which means that the atom of sublattice \( o \) in the unit cell with the origin is transferred to the site of sublattice \( \delta \) in the unit cell at the position \( u_o \) (e.g., for \( \pi/3 \) rotation, see Fig. (1d)). The values of indices \( \delta \) and vectors \( u_o \) for representative operations are shown in Table II.

![FIG. 1. (Color online) Honeycomb lattice, its Brillouin zone, Bravais lattice vectors in the bases, and illustration of \( \pi/3 \) rotation. (a) Lattice structure. The \( A(B) \) sublattice is indicated by red (blue) spheres. The primitive vectors of the lattice are \( a_1, a_2 \) and a unit cell is the pentagon enclosed with grey line. (b) Brillouin zone. The grey part is the irreducible region of Brillouin zone. (c) Bravais lattice vectors \( R_m \) in the 13 plane-wave bases \( f_m(p) = e^{i R_m \cdot p} \) used by us. (d) Transfer of \( A, B \) sites upon \( \pi/3 \) rotation followed by appropriate shift.](image)
Corresponding symmetry relations for the bosonic propagators read
\[
P_{(C,D)\tilde{\alpha}_1,\tilde{\alpha}_2,m,\tilde{\alpha}_3,n}(q) = P_{(C,D)\tilde{\alpha}_3,n,\tilde{\alpha}_2,m,\tilde{\alpha}_1}(q)^* \quad \text{(PHS),} \tag{24}
\]
\[
P_{\tilde{\alpha}_1,\tilde{\alpha}_2,m,\tilde{\alpha}_3,n}(q) = e^{i\mathbf{q} \cdot (\mathbf{R}_m - \mathbf{R}_n)} \times P_{\tilde{\alpha}_2,\tilde{\alpha}_1,-\mathbf{R}_m,\mathbf{R}_n}(q) \quad \text{(RAS),} \tag{25}
\]
\[
C_{(D)}\tilde{\alpha}_1,\tilde{\alpha}_2,m,\tilde{\alpha}_3,n(q) = e^{i\mathbf{q} \cdot (\mathbf{R}_n - \mathbf{R}_m)} \times C_{(D)}\tilde{\alpha}_3,n,-\mathbf{R}_m,\tilde{\alpha}_2,\tilde{\alpha}_1,-\mathbf{R}_n(-q) \quad \text{(RAS).}
\]

### B. Estimation of order parameters

There are several methods to determine the leading instabilities and the momentum dependence of corresponding order parameters. In early FRG analyses, it has been a common implementation to assume the initial form of the order parameters and trace the RG flow of the order parameters and susceptibilities\textsuperscript{21,27,31}. The renormalized order parameters depend on their initial choice of the momentum dependence, and therefore these studies do not present an unbiased tool to determine the form factor of the order parameters. It makes the problem cumbersome to postulate all possibility of the initial form of the order parameters, especially for the case of the multi-band models. Thus, in later FRG studies addressing multi-band models, the effective interaction in the particular ordering channel is decomposed into different eigenmode contributions and the eigenfunction corresponding to most diverging eigenvalue is estimated to be the form factor of the order parameter in the channel\textsuperscript{24,26,32,35}. We identify the form factor of order parameters by considering the linear response of the system to virtual infinitesimal external fields coupled to the fermion bilinears\textsuperscript{36}.

For the singlet and triplet pairings, we can add the following Hamiltonians in momentum space, respectively,
\[
H_{\text{SFC}} = -\frac{\lambda}{2} \sum_{\sigma} S_{\sigma\sigma}(k, q - k) \cdot c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{q} - \mathbf{k},\sigma} \cdot c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{q} - \mathbf{k},\sigma}^\dagger + \text{c.c.}, \tag{26}
\]
\[
H_{\text{SC}} = -\frac{\lambda}{2} \sum_{\sigma} T_{\sigma\sigma}(k, q - k) \cdot c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{q} - \mathbf{k},\sigma} c_{\mathbf{q} - \mathbf{k},\sigma}^\dagger + \text{c.c.}, \tag{27}
\]
in which the coupling constants \(S_{\sigma\sigma}(k, q - k)\) and \(T_{\sigma\sigma}(k, q - k)\) have the following relations:
\[
S_{\sigma\sigma}(k, q - k) = S_{\sigma\sigma}(q - k, k),
\]
\[
T_{\sigma\sigma}(k, q - k) = -T_{\sigma\sigma}(q - k, k). \tag{28}
\]
Now, we briefly describe how the form factor of order parameter in singlet paring channel can be estimated.
The additional action corresponding to Eq. (20) is
\[
S_\lambda = -\frac{\lambda}{2} \left[ \sum_{o,o',l,\sigma} C^*_{o,o',l,\sigma} \bar{\psi}_\sigma(l,o) \bar{\psi}_{-\sigma}(q - l, o') + \sum_{o,o',l,\sigma} C_{o,o',l,\sigma} \psi_{-\sigma}(q - l, o') \psi_{\sigma}(l, o) \right]
\] (29)

where the index \( l \) contains the wavevector \( k \) and Matsubara frequency \( \omega \), i.e., \( l = (\omega, k) \), and coupling constant \( C_{o,o',l,\sigma} \) is \( C_{o,o',l,\sigma} = \sigma S_{\omega o}(k, q - k) \).

The order parameter in the singlet pairing channel is
\[
\Delta^\text{SC}_{\omega o}(k, q - k) \equiv \lim_{\lambda \to +0} \sum_{\sigma} \langle c^\dagger_{k,o,\sigma} c_{k-o',-\sigma} \rangle \lambda
\] (30)

where \( \langle \cdot \rangle \lambda \) means average in the grand canonical ensemble with the action including additional term in Eq. (29).

\[
\langle O \rangle \lambda = \frac{\int \prod d\bar{\psi}_\sigma(\xi) d\psi_\sigma(\xi) e^{-[S(\bar{\psi}, \psi) + S_{\lambda}(\bar{\psi}, \psi)]}}{\int \prod d\bar{\psi}_\sigma(\xi) d\psi_\sigma(\xi) e^{-[S(\bar{\psi}, \psi) + S_{\lambda}(\bar{\psi}, \psi)]}}
\] (31)

When the system has no long-range order, the order parameter \( \Delta^\text{SC}_{\omega o}(k, q - k) \) in Eq. (30) vanishes. However, when the system is approaching the critical point, the corresponding susceptibility diverges and the order parameter can develop. We postulate that the system has no long-range order, and consider the quantity
\[
\Delta^\lambda_{\omega o}(k, q - k) \equiv \lim_{\lambda \to +0} \sum_{\sigma} \langle c^\dagger_{k,o,\sigma} c^\dagger_{k-q,-\sigma} \rangle \lambda
\] (32)

Taking into account the vanishing of \( \Delta^\lambda_{\omega o}(k, q - k) \) at \( \lambda = 0 \) and Taylor expanding Eq. (32) with respect to \( \lambda \), we have
\[
\Delta^\lambda_{\omega o}(k, q - k) = \frac{\lambda}{2} \sum_{\sigma, \omega, \omega'} \sum_{\nu, \nu', l, l', \sigma'} C_{\nu,\nu',l,l',\sigma'} \times
\langle \bar{\psi}_\sigma(l, o) \bar{\psi}_{-\sigma}(q - l, o') \bar{\psi}_{-\sigma}(q - l', \nu') \bar{\psi}_{\sigma}(l', \nu) \rangle \lambda = 0.
\]

Using the relation between the 4-point Greens function and the effective interaction\(^\text{27}\) and taking an approximation of \( G_{\omega o}(\omega, k) \approx G^0_{\omega o}(\omega, k) \), we obtain the following result
\[
\Delta^\lambda_{\omega o}(k, q - k) = 2\lambda \sum_{\mu, \mu'} L_{\mu o,\mu' o'}(k, q - k) S_{\mu \mu'}(k, q - k)
- 2\lambda \sum_{\nu, \nu', \rho, \rho', \mu, \mu'} \frac{1}{S_{BZ}} \int dk' S_{\nu \nu'}(k', q - k')
\times L_{\nu \nu', \rho \rho'}(k', q - k') L_{\mu \mu', \rho' \rho''}(k, q - k)
\times V_{\nu \rho', \mu' \rho''}(q - k', k' - k, k, q - k, k, k)
\] (32)

where \( V_{\nu \rho', \mu' \rho''}(k_1', k_2', k_1, k_2) \) is the effective interaction,
\[
V_{\nu \rho', \mu' \rho''}(k_1', k_2', k_1, k_2) = \lim_{\Omega \to 0} V_{\Omega}^{\nu \rho', \mu' \rho''}(k_1', k_2', k_1, k_2),
\]

and \( L_{\mu o,\mu' o'}(k, q - k) \) is defined as
\[
L_{\mu o,\mu' o'}(k, q - k) \equiv \frac{1}{\beta} \sum \omega G^0_{\omega o}(\omega, k) G^0_{\omega' o'}(-\omega, q - k).
\]

Eq. (32) can be represented schematically as in Fig. 2(a) and is equivalent to the renormalization of the vertex \( S_{\mu \mu'}(k, q - k) \) shown in Fig. 2(b). The renormalization in Fig. 2(b) is consistent with Fig. 1 in Ref. 28 where the form factors of order parameters is analyzed using the Bethe-Salpeter equation.

![Diagram](a)

![Diagram](b)

FIG. 2. (a) A schematic representation of the order parameter \( \Delta_{\omega o}(k, q - k) \). The left diagram in the bracket stands for the order parameter. (b) The renormalization of the vertex \( S_{\mu \mu'}(k, q - k) \). The vertex with the grey arc is the renormalized three-point vertex, while that with the white arc is the bare vertex \( S_{\mu \mu'}(k, q - k) \).

In the limit of \( \lambda \to +0 \), the first term in the right hand side of Eq. (32) vanishes, while the second term may have finite value due to a divergence of the effective interaction. So, replacing \( k \) with \( k + q \) in Eq. (32) we get
\[
\lim_{\lambda \to +0} \Delta^\lambda_{\omega o}(k + q, -k) = -2\lambda \sum_{\nu, \nu', \rho, \rho', \mu, \mu'} \frac{1}{S_{BZ}} \int dk' S_{\nu \nu'}(k' + q, -k')
\times L_{\nu \nu', \rho \rho'}(k' + q, -k'; k + q, -k) L_{\mu \mu', \rho' \rho''}(k + q, -k).
\] (33)

We can rewrite \( L_{\nu \nu', \mu' \mu''}(k' + q, -k'; k + q, -k) \) in terms of \( V_{\nu \rho', \mu' \rho''}(q - k', k' - k, k, q - k, k, k) \) by inverting Eq. (11).

By Fourier transforming Eq. (30), we can get the order parameter in real space.
\[
\Pi^\text{SC}_{\omega o}(R_i, R_i - R_o) = \lim_{\lambda \to +0} \sum \sigma \langle c^\dagger_{R_i, o, \sigma} c_{R_i - R_o, -\sigma} \rangle \lambda
= \sum_{\sigma} e^{-i q R} \lim_{\lambda \to +0} \int dk f^\dagger_\sigma(k) \Delta^\lambda_{\omega o}(k + q, -k)
\]

where \( R \) and \( q \) are the integration variables.
Using Eq. (33) and introducing $S_{\alpha\alpha'}m(m)$ by $S_{\alpha\alpha'}(k + q, -k) = \sum_{\mu,\mu'} S_{\mu\mu'm}(q)f_{\mu'}(k)$, we obtain the following expression for the order parameter,

$$
\Pi^{SC}(R_i, R_i - R_\alpha) = -2\lim_{\lambda \to +0} \lambda \sum_q e^{-i\mathbf{q}\cdot\mathbf{R_i}} \times \sum_{\mu,\mu'} S_{\mu\mu'm}(q) \cdot [\chi^{pp}(q)V^{P}(q)\chi^{pp}(q)]_{\mu\mu',m,\alpha\alpha'},
$$

where $\chi^{pp}(q)$ is

$$
\chi^{pp}_{\alpha\beta\alpha'\beta'}(q) = -\frac{1}{S_{BZ}} \int dk f_{m}(k)f_{n}(k) \chi^{pp}(q) 
\times \frac{1}{\beta} \sum_{\omega} G_{\alpha\alpha'}^{0}(\omega, k + q) G_{\beta\beta'}^{0}(\omega, -k),
$$

If there is only one pairing mode emerged with the transfer momentum $Q$, the sum $\sum_q$ in Eq. (33) is removed and $q$ is replaced with $Q$. We can use the eigenvalues $\lambda_i(Q)$ and eigenvectors $\phi^{\beta}_{\alpha\alpha'}(Q)$ to decompose the following Hermitian matrix,

$$
W^{SC}_{\phi^{\beta}_{\alpha\alpha'}m,m,\alpha\alpha'}(Q) \equiv [\chi^{pp}(q)V^{P}(q)\chi^{pp}(q)]_{\alpha\beta\alpha'\beta'}(Q)
$$

$$
\lambda_i(Q) [\sum_{\mu,\mu'} S_{\mu\mu'm}(Q) \phi^{\beta}_{\alpha\beta}(Q)] \cdot \phi^{\alpha}_{\alpha'\alpha'}(Q)^*,
$$

which means

$$
\Pi^{SC}(R_i, R_i - R_\alpha) = C e^{-iQ\cdot R_i} \phi^{\alpha}_{\alpha\alpha'}(Q)^*.
$$

When several eigenvalues are similarly dominant in FRG flow, the system may have no long-range order due to competition effects between the different ordering tendencies. For the case of triplet pairing, all the results above are valid except for different symmetry relations of eigenvectors:

$$
\phi^{\alpha}_{\alpha'\alpha} = e^{iQ\cdot R_i}\phi^{\alpha}_{\alpha'\alpha},
$$

for singlet pairing,

$$
\phi^{\alpha}_{\alpha'\alpha} = -e^{iQ\cdot R_i}\phi^{\alpha}_{\alpha'\alpha},
$$

for triplet pairing,

where $\alpha$ is the index of plane-wave base with vector $-R_\alpha$.

The form factors of order parameters in spin and charge channels can be obtained in a similar way and have nearly identical structures. The matrix $W^{SC}(Q)$ in Eq. (33) is changed into following matrices, $W^{SPN}(Q)$ for spin channel and $W^{CHG}(Q)$ for charge channel, respectively,

$$
W^{SPN}(Q) = \chi^{ph}(Q)V^{P}(Q)\chi^{ph}(Q),
$$

$$
W^{CHG}(Q) = \chi^{ph}(Q)V^{C}(Q)\chi^{ph}(Q),
$$

Here $\chi^{ph}(q)$ is

$$
\chi^{ph}_{\alpha\alpha'}m,m,\alpha\alpha'(q) = -\frac{1}{S_{BZ}} \int dk f_{m}(k)f_{n}(k) \chi^{ph}(q) 
\times \frac{1}{\beta} \sum_{\omega} G_{\alpha\alpha'}^{0}(\omega, k + q) G_{\beta\beta'}^{0}(\omega, -k).
$$

The order parameters in real space are defined as

$$
\Pi^{SC}(R_i, R_i - R_\alpha) = \lim_{\lambda \to +0} \sum_{\alpha} \langle c_{R_i,\alpha\alpha'}^{\dagger}c_{R_i-R_\alpha\alpha'}^{\dagger}\alpha\alpha'^{\dagger}\rangle_{\lambda}
$$

for triplet pairing channel,

$$
\Pi^{SPN}(R_i, R_i - R_\alpha) = \lim_{\lambda \to +0} \sum_{\alpha} \langle c_{R_i,\alpha\alpha'}^{\dagger}c_{R_i-R_\alpha\alpha'}^{\dagger}\alpha\alpha'^{\dagger}\rangle_{\lambda}
$$

for spin channel,

$$
\Pi^{CHG}(R_i, R_i - R_\alpha) = \lim_{\lambda \to +0} \sum_{\alpha} \langle c_{R_i,\alpha\alpha'}^{\dagger}c_{R_i-R_\alpha\alpha'}^{\dagger}\alpha\alpha'^{\dagger}\rangle_{\lambda}
$$

for charge channel.

Similarly to Eq. (37), the form factor in the spin (charge) channel is given by

$$
\Pi^{SPN(CHG)}(R_i, R_i - R_\alpha) =
$$

$$
C e^{-iQ\cdot R_i}\phi^{\alpha}_{\alpha\alpha'}(Q)^* + C^* e^{iQ\cdot R_i-R_\alpha}\phi^{\alpha}_{\alpha\alpha'}(Q),
$$

where $\phi^{\alpha}_{\alpha\alpha'}(Q)$ is the eigenvector of the dominantly divergent eigenmode of the matrix $W^{SPN}(Q)$ ($W^{CHG}(Q)$) in the spin (charge) channel.

IV. RESULTS AND DISCUSSION

Fourier transforming and diagonalizing the single-particle Hamiltonian, Eq. (2), we obtain the one-particle energy and transformation matrix in Eq. (12),

$$
E_1(k) = -|d(k)|, E_2(k) = +|d(k)|,
$$

$$
T_{ab}(k) = \frac{d(k)}{|d(k)|}\frac{d(k)}{|d(k)|}.
$$

with $d(k) = t(1 + 2\cos k_\perp e^{-i\sqrt{\frac{1}{2}}k_\perp}).$ The initial values of projections, $V^{P}(0)(Q)$, $V^{C}(0)(Q)$, and $V^{D}(0)(Q)$, are obtained by Fourier transforming the interaction Hamiltonian in Eq. (3) and projecting it onto the three channels via Eq. (11). The expressions of these values are
considerably simple in the orbital picture.

\[
V_{AA0,AA0}^{P(0)}(q) = V_{BBO,BBO}^{P(0)}(q) = U, \\
V_{AA0,AA0}^{D(0)}(q) = V_{BBO,BBO}^{D(0)}(q) = U + V_2 \sum_{j=1}^{6} e^{i q R_j}, \\
V_{AAm,AAm}^{P(0)}(q) = V_{BBOm,BBOm}^{P(0)}(q) = V_2 (m = 1 \sim 6), \\
V_{ABBO,ABBO}^{P(0)}(q) = V_{BBOm,ABBO}^{P(0)}(q) = J, \\
V_{ABm,BAm}^{P(0)}(q) = [V_{ABm,BAm}^{P(0)}(q)]^* = J e^{-i q R_m} (m = 2, 3), \\
V_{ABm,BAm}^{P(0)}(q) = [V_{BBOm,AA0}^{P(0)}(q)]^* = J (1 + e^{-i q R_2} + e^{-i q R_3}), \\
V_{ABm,BAm}^{D(0)}(q) = J (m = 0, 2, 3), \\
V_{ABm,BAm}^{D(0)}(q) = J (m = 0, 5, 6), \\
\text{All other elements} = 0.
\]

In the current implementation of TUFGRG, the matrices \(P, C, D, V^P, V^C, V^D, \chi^{pp}, \chi^{ph}\) have 52 \(\times\) 52 structures. The flow equation for the bosonic propagators, Eq. (44) is solved for the transfer momenta in the irreducible region of BZ shown in Fig. (3a) and Fig. (3b). The discretized transfer momenta are distributed where the ordering vectors are expected. Fig. (3c) shows the sampling momenta used for the integration of \(\chi^{pp}\) and \(\chi^{ph}\) in Eq. (44), which are denser near the Dirac points \(K\) and \(K'\). This \(k\)-mesh is obtained in a similar way as in Ref. [20].

The different tendencies towards symmetry broken ground states are identified via the estimation method in Sec. III B. We have analyzed these tendencies by varying the interaction parameters \(V_2, J\), while fixing the on-site repulsion \(U\). The results are summarized in tentative phase diagrams shown in Fig. 4. The critical scales \(\Omega_c\), at which these transitions may occur, are also provided using the colorbar. We explain the instabilities appearing in the phase diagram below.

- **AFM** – Antiferromagnetic spin-density-wave instability

It is known that the on-site repulsion exceeding a critical value \(U_C \approx 3.8t\) drives the antiferromagnetic (AFM) spin-density-wave instability for the half-filled Hubbard model on the honeycomb lattice[13]. This instability is manifested in the RG flow as a dominantly divergent eigenmode of \(W^{SPN}(Q = 0)\) which has real numbers \(\phi_{AA0}\) and \(\phi_{BBO}\) with a relation \(\phi_{AA0} = -\phi_{BBO}\) as its largest components. The relation \(\phi_{AA0} = -\phi_{BBO}\) represents the staggered spin configuration on the \(A\) and \(B\) sublattices. The AFM instability occurs only for dominant \(U\) (\(U = 5.0t\) in Fig. 3) and vanishes by inclusion of small \(J\). The vanishing of the AFM by small \(J\) implies that the exchange interaction \(J\) has strong tendency to destroy AFM and recover the semi-metallic (SM) phase. As you see in Fig. 3 the inclusion of the parameter \(J\) smaller than 1.5\(t\) has no impact on the emergent phases for \(U = 0\), which is supposed to be due to two competing ordering tendencies of the parameter \(J\), i.e., the pairing and ferromagnetic tendencies. Involving \(V_2\) larger than

![FIG. 3. (a) Mesh of \(N_q = 171\) points for transfer momenta within the irreducible region of BZ in the particle-particle channel. The points are distributed denser near the \(\Gamma\) point. The bosonic propagators \(P(q)\) are calculated for these points. (b) Mesh of \(N_q = 175\) points for transfer momenta within the irreducible region of BZ in the particle-hole channel. The points are distributed denser near the \(\Gamma\) and \(K\) points. The bosonic propagators \(C(q)\) and \(D(q)\) are calculated for these points. (c) Mesh of \(N_k = 8280\) points for sampling momenta used in the integration of \(\chi^{pp}\) and \(\chi^{ph}\). The points are distributed denser near the Dirac points \(K\) and \(K'\).](image-url)
magnetic (FM) spin-density-wave instability for $U = 5.0t$ but not for $U = 0$. This fact can be explained by duality of the effect of the exchange interaction $J$; the ferromagnetic exchange that promotes the spin alignment and the pair hopping that drives the superconducting pairing. When $U = 5.0t$, the large value of the on-site repulsion $U$ blocks the pair hopping and permits only the ferromagnetic exchange. The ferromagnetic exchange ultimately wins the AFM ordering tendency by the parameter $U$ and produces the FM ordered phase when increasing the parameter $J$. However, for the case of zero on-site repulsion, the absence of the Coulomb blockade effect induces the competition between the ferromagnetic exchange and pair hopping, thus suppressing the FM order.

- **QSH – Quantum spin hall instability**

The quantum spin Hall (QSH) phase is the most tempting one in the phase diagram in Fig. 4. The existence of this phase remains an inclusive problem. The QSH instability is characterized by following dominantly divergent eigenmode of $W^{\text{SPN}}(Q = 0)$,

$$
\phi_{AA1} = -\phi_{AA2} = \phi_{AA3} = -\phi_{AA4} = -\phi_{AA5} = -\phi_{AA6} = -iR,
\phi_{BB1} = -\phi_{BB2} = \phi_{BB3} = -\phi_{BB4} = \phi_{BB5} = -\phi_{BB6} = iR,
$$

with a real constant $R$. This form factor corresponds to an ordered pattern of spin currents shown in Fig. 5a. We have not found the QSH instability in the absence of the exchange interaction $J$, which is consistent with previous TUFGRG result. In our study it occurs in a relatively narrow region of the parameter space, namely around $U \approx 0, V_2 \approx t, J = 2t \sim 4t$. We performed test calculations in which we involved only the pair hopping or the ferromagnetic exchange, separately, keeping the

2.5$t$ also induces the vanishing of AFM, but it makes another charge-density-wave order develop. The SM phase is stable in an extended region implying a suppression of spin or charge order due to competition effects between the different ordering tendencies.

- **FM – Ferromagnetic spin-density-wave instability**

This instability is manifested in the RG flow as a dominantly divergent eigenmode of $W^{\text{SPN}}(Q = 0)$ which has real numbers, $\phi_{AA0} = \phi_{BB0}$ as its largest components. Increased parameter $J$ larger than 2.8$t$ drives the ferromagnetic spin-density-wave instability for $U = 5.0t$ but not for $U = 0$. This fact can be explained by duality of the effect of the exchange interaction $J$; the ferromagnetic exchange that promotes the spin alignment and the pair hopping that drives the superconducting pairing. When $U = 5.0t$, the large value of the on-site repulsion $U$ blocks the pair hopping and permits only the ferromagnetic exchange. The ferromagnetic exchange ultimately wins the AFM ordering tendency by the parameter $U$ and produces the FM ordered phase when increasing the parameter $J$. However, for the case of zero on-site repulsion, the absence of the Coulomb blockade effect induces the competition between the ferromagnetic exchange and pair hopping, thus suppressing the FM order.

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\phi_{BB1} = -\phi_{BB2} = \phi_{BB3} = -\phi_{BB4} = \phi_{BB5} = -\phi_{BB6} = iR,
$$

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![FIG. 4. (Color online) Dominant instabilities for different interaction parameters. The colorbar indicates the value of the critical scales $\Omega_c$ at which the corresponding transitions may occur. In the region marked with SM, there is no divergence of any bosonic propagator in the RG flow down to the stopping scale $\Omega^* = 10^{-4}t$. In the region marked with N/A, there is a divergence of some bosonic propagator, however, different ordering tendencies coexist and compete with each other, so that a clear identification of the leading instability is not possible and the divergent $W^{\text{SC}}(Q), W^{\text{SPN}}(Q)$ or $W^{\text{CHG}}(Q)$ at $\Omega_c$ shows a mix of various instabilities.](image)

![FIG. 5. (Color online) Representative spin current and bond strength patterns for the quantum spin Hall phase and spin-Kekulé phase. (a) Spin current pattern in the quantum spin Hall phase. The arrows indicate the directions of the spin currents. (b) Spin bond strength pattern in the spin-Kekulé phase. The red (blue) lines represent the positive (negative) values of spin bond order parameters and the line widths indicate their magnitudes. A unit cell is shown as the region enclosed with grey line.](image)
values of $J$ and $V_2$ unchanged. Involving only one effect did not drive the QSH order, which demonstrated that a combination of pair hopping and ferromagnetic exchange is essential for the emergence of QSH. Since the density-density repulsion $V_2$ is generally larger than the exchange integral $J$, the region of QSH phase is far from reality. The large value of $J$ can affect the validity of the weak coupling FRG approach and damage the reliability of the result. However, we expect that our results could shed some light on the issue of the existence of QSH state.

- **SK – Spin Kekulé bond order instability**

This instability is manifested in the RG flow as following divergent eigenmode of $W_{\text{SPN}}(Q = K)$ in the spin channel,

$$
\phi_{AB0} = R, \phi_{BA0} = R, \phi_{AB2} = \phi_{BA5} = R \cdot e^{-i\phi}, \quad \phi_{AB3} = \phi_{BA6}^* = R \cdot e^{i\phi}
$$

which represents a spin bond order with an enlarged unit cell, as shown in Fig. 6(b). This order can be thought of as the spinful counterpart of the Kekulé bond order. The spin-Kekulé (SK) phase has been proposed theoretically in previous studies. Its unit cell is three times bigger than the original one and contains six atoms in it. Despite our current Hamiltonian is capable of producing this exotic spin-Kekulé phase, the fact that it is emerged only in one segment of our phase diagram with dominant $J$ ($U \approx 0$, $V_4 \approx 0.5t$, $J \approx 3.5t$) casts some doubt on this result. We cannot exclude the possibility that the SK phase might be an artifact generated by the enhancement of exchange integral.

- **CDW$_3$ – Three-sublattice charge-density-wave instability**

Large part of our phase diagrams is occupied by CDW phase named as three-sublattice charge density wave (CDW$_3$) which has the enlarged unit cell as for the spin-Kekulé phase. Especially, for the case of $U = 0$, the CDW$_3$ phase develops in the major part of the phase diagram. It is driven by the next-nearest-neighbor repulsion $V_2$ exceeding a critical value and characterized by following two degenerate divergent eigenmodes of $W_{\text{CHG}}(Q = K)$ in the charge channel,

$$
\phi_{AA0}^3 = R, \phi_{BB0}^3 = 0, \text{ and } \phi_{AA0}^2 = 0, \phi_{BB0}^2 = R.
$$

These two form factors are represented by the charge ordering patterns shown in Fig. 6 and these four patterns will be linearly superposed to construct the charge density distribution in real space. To determine their superposition in detail, one needs to perform the mean-field calculation or the analysis beyond the linear response, but these are beyond the scope of the present work.

The low-energy effective Hamiltonian becomes

$$
H_{\text{CDW}_3} = -\frac{1}{N} \sum_{\sigma} V \left( N_{K}^{\sigma} N_{K}^{-\sigma} + N_{-K}^{\sigma} N_{-K}^{-\sigma} \right)
$$

where $N_{K}^\sigma = \sum_{k,\sigma} c_{k+K,\sigma}^\dagger c_{k,\sigma}$ and $V$ is a positive constant. Unlike the effective Hamiltonian in Ref. 14, Eq. 48 has no coupling between different orbital indices. Even when properly involving the nearest-neighbor repulsion $V_1$, the form of the low-energy effective Hamiltonian in Eq. 48 is retained. This disagreement can be attributed to the so-called *orbital makeup* in the band picture.

- **iCDW – Incommensurate charge-density-wave instability**

When increasing the parameter $J$, the CDW$_3$ phase changes to incommensurate charge-density-wave (iCDW) phase. The ordering vector depends on the value of $V_2$ and $J$, wandering near the $K$ point. The iCDW phase is firstly reported in Ref. 14. It is manifested in the RG flow as following divergent eigenmode of $W_{\text{CHG}}(Q = Q_0)$ in the charge channel,

$$
\phi_{AA0}^1 = R \cdot e^{i\Delta \phi}, \phi_{BB0}^1 = -R \cdot e^{-i\Delta \phi}
$$

which gives the charge distribution,

$$
N_{R_1}^A = N_0 + \Delta N \cdot \cos(Q_0 \cdot R_1 + \varphi_0 + \Delta \phi),
N_{R_1}^B = N_0 - \Delta N \cdot \cos(Q_0 \cdot R_1 + \varphi_0 - \Delta \phi).
$$

In the transition from the CDW$_3$ to iCDW phase, the degeneracy will change from two to one and the ordering vector will also change gradually near the $K$ point. It would be interesting to investigate the behavior of this transition in detail, which we leave for future work.
V. CONCLUSION

In this work we have investigated the effect of enhanced exchange interaction on possible ground-state orderings of electrons on the honeycomb lattice at half-filling. In order to calculate the effective interactions and analyze the ground states for the system, we have employed the TUFGRG scheme with high resolution of wave-vector dependences in the effective interaction. The ground-state phase diagrams in the space of next-nearest-neighbor repulsion and nearest-neighbor exchange integral are obtained for two typical values of on-site repulsion, namely, for \( U = 0 \) and \( U = 5t \). Inclusion of the exchange interaction produces the phase diagram with diverse ordering tendencies, especially for vanishing on-site repulsion. The commensurate CDW order, i.e. the CDW\(_3\) order has developed in wide region of the diagram, which is replaced by the incommensurate CDW order when increasing the exchange integral. The topological QSH state is emerged in a relatively narrow region of the parameter space around \( U \approx 0, V_2 \approx t, J \approx 2t \sim 4t \). This phase is induced by a combination of the ferromagnetic exchange and pair hopping interactions. Through test calculation, we verified that involving only the pair hopping or the ferromagnetic exchange would not produce the QSH phase. There exists another interesting phase named spin-Kekulé phase in a very small part of the parameter space near \( U \approx 0, V_2 \approx 0.5t, J \approx 3.5t \) but it is suspected to be an artifact of the TUFGRG calculation due to very limited region of existence and too large value of exchange integral. For the case of \( U = 5t \), there also exist the antiferromagnetic and ferromagnetic phases for small and large value of the parameter \( J \), respectively, but these phases change into CDW\(_3\) by increase of parameter \( V_2 \). There is strong competition between different ordering tendencies, which renders the semi-metallic phase stable in relatively wide regions of the phase diagrams. Any signal for a dominating pairing instability has not been found at half-filling as in previous results.

In addition, we derived the symmetry relations of the bosonic propagators and proposed the linear-response based approach for identifying the type of order. The former can efficiently reduce the computational effort for the systems with high geometrical symmetry and the latter can reasonably and quickly determine the form factors of order parameters.

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