Alleviating the Sign Problem in Quantum Monte Carlo Simulations of Spin-Orbit-Coupled Multi-Orbital Hubbard Models

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We present a strategy to alleviate the sign problem in continuous-time quantum Monte Carlo (CTQMC) simulations of the dynamical-mean-field-theory (DMFT) equations for the spin-orbit-coupled multi-orbital Hubbard model. We first identify the combinations of rotationally invariant Hund coupling terms present in the relativistic basis which lead to a severe sign problem. Exploiting the fact that the average sign in CTQMC depends on the choice of single-particle basis, we propose a bonding-antibonding basis ($V_{3/2BA}$) which shows an improved average sign compared to the widely used relativistic basis for most parameter sets investigated. We then generalize this procedure by introducing a stochastic optimization algorithm that exploits the space of single-particle bases and show that $V_{3/2BA}$ is very close to optimal within the parameter space investigated. Our findings enable more efficient DMFT simulations of materials with strong spin-orbit coupling.

**Introduction.**- Spin-orbit coupling (SOC) is an essential ingredient in the study of exotic phases in correlated electron systems [1], such as unconventional superconductivity in 4d transition-metal oxides [2,3], topological phases of matter in quantum spin-Hall insulators [10-12], excitonic insulators [13,14] or Kitaev-model-based insulators [15,23], to mention a few. A prototypical minimal model that includes the interplay between spin-orbit coupling and correlations is the relativistic multi-orbital Hubbard model. Its non-relativistic counterpart has been intensively investigated in the past and shows a rich phase diagram [14,24-26]. The relativistic multi-orbital Hubbard model [15,17,27], however, is much less understood since the choice of algorithms is strongly limited due to the extra computational complications associated with (multi-)spin-orbit-coupled degrees of freedom.

One of the promising formalisms to investigate the Hubbard model and its generalizations is the dynamical mean-field theory (DMFT) [28,29] that has provided important insights into multi-orbital physics also in combination with ab-initio calculations for real materials [30,32]. The continuous-time quantum Monte Carlo method (CTQMC) [33], particularly the hybridization expansion algorithm (CTHYB) [34,35] is the most widely used impurity solver in multi-orbital DMFT calculations. However, CTHYB suffers from the notorious sign problem when the SOC is included in the calculations. The sign problem grows exponentially with inverse temperature [36,37], and typically prevents the study of low-temperature symmetry-broken phases. Alleviating the sign problem in CTHYB would help improve our understanding of phenomena determined by the interplay of spin-orbit coupling and correlations [2,15,38,39].

For Quantum Monte Carlo (QMC) algorithms based on auxiliary fields, there have been various successful advances which unveil the origin of the sign problem and suggest a solution in many cases [10,48], including the recently developed idea of Majorana symmetry [49,51]. The rotationally invariant Hund coupling in the SO-coupled multi-orbital Hubbard system, however, generates rather complex interaction terms. Furthermore, the non-local-in-time expansion scheme of CTHYB makes it difficult to track the origin of the fermionic sign on the worldline configuration.

In this letter, we systematically study the nature of the sign problem of the CTHYB for the SO-coupled three-orbital Hubbard model and propose a strategy to alleviate it. We employ a numerical sign-optimization scheme, called spontaneous perturbation stochastic approximation (SPSA) [52], to determine the optimal basis in terms of average sign. Remarkably, this optimal basis can be well approximated by a simple one, which we denote as $V_{3/2BA}$. The $V_{3/2BA}$ basis is obtained from the relativistic basis by a bonding-antibonding transformation.

**Model and Method.**- Our model Hamiltonian is composed of the three terms

\[ \mathcal{H} = \mathcal{H}_{t} + \mathcal{H}_{soc} + \mathcal{H}_{int}, \]  

(1)

where $\mathcal{H}_{t}$, $\mathcal{H}_{soc}$, and $\mathcal{H}_{int}$ are, respectively, the electron hopping, SOC, and Coulomb interaction terms. For the noninteracting electron hopping part we assume a degenerate semi-circular density of states $\rho(\omega) = (1/\pi D)\sqrt{1-(\omega/D)}^{2}$ and set the half-bandwidth $D$ as the unit of energy. In the orbital-spin basis ($V_{os}$), $\mathcal{H}_{SOC}$ has the form

\[ \mathcal{H}_{soc} = -\lambda \sum_{i,\alpha,\sigma} c_{i\alpha\sigma}^{\dagger} (\alpha \sigma | \mathbf{L}_{eff} \cdot \mathbf{S} | \alpha' \sigma') c_{i\alpha'\sigma'}, \]  

(2)

where $\mathbf{L}_{eff}$ is the $l = 1$ orbital angular momentum operator and $\mathbf{S}$ is the spin operator. $c_{i\alpha\sigma}$ ($c_{i\alpha\sigma}^{\dagger}$) is the electron annihilation (creation) operator of orbital $\alpha$ ($yz, zx, xy$).
and spin $\sigma (\uparrow, \downarrow)$ at lattice site $i$. We introduce the Slater-Kanamori form of the Coulomb interaction including the spin-flip and pair-hopping terms:

$$H_{\text{int}} = U \sum_{i,\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} + \sum_{i,\alpha<\alpha'} (U' - J_H \delta_{\sigma\sigma'}) n_{i\alpha\sigma} n_{i\alpha'\sigma'}$$

$$-J_H \sum_{i,\alpha<\alpha'} (c_{i\alpha\uparrow} c_{i\alpha'\downarrow} + h.c.) + J_H \sum_{i,\alpha<\alpha'} (c_{i\alpha\uparrow} c_{i\alpha'\downarrow} + h.c.) . \quad (3)$$

Here, $U$ ($U'$) is the intra- (inter-)orbital Coulomb repulsion, and $J_H$ is the strength of the Hund coupling. To make $H_{\text{int}}$ rotationally invariant, $U' = U - 2J_H$.

We solve the model using DMFT, where the lattice model is mapped onto a quantum impurity model by means of a self-consistency relation. CTHYB solves the quantum impurity model via an expansion of the partition function in powers of the hybridization function. Since the impurity partition function is expressed as a weighted sum $Z_{\text{imp}} = \sum_\omega \omega(x)$, a potential sign problem appears when the weight $\omega(x)$ in the QMC for certain configurations $x$ becomes negative. The severity of the sign problem depends on the average sign

$$(\text{sign}) = \frac{\sum_x \text{sign}(\omega(x)) |\omega(x)|}{\sum_x |\omega(x)|} . \quad (4)$$

An important aspect to keep in mind is that the sign problem depends on the single-particle basis. For example, it has been reported that if the electron operators $(\tilde{c}_{j,m})$ are expressed in the relativistic $j_{\text{eff}}$ basis ($V_{\text{eff}}$),

$$\begin{pmatrix}
\tilde{c}_{\frac{1}{2},+\frac{1}{2}} \\
\tilde{c}_{\frac{3}{2},+\frac{1}{2}} \\
\tilde{c}_{\frac{3}{2},-\frac{1}{2}} \\
\tilde{c}_{\frac{5}{2},-\frac{1}{2}}
\end{pmatrix} = \frac{1}{\sqrt{6}} \begin{pmatrix}
-\sqrt{2} + i\sqrt{2} \\
-1 \\
-i \sqrt{3} \\
0
\end{pmatrix} \begin{pmatrix}
c_{y\downarrow} \\
c_{x\downarrow} \\
c_{x\uparrow} \\
c_{y\uparrow}
\end{pmatrix} ,$$

$$\begin{pmatrix}
\tilde{c}_{\frac{5}{2},-\frac{1}{2}} \\
\tilde{c}_{\frac{7}{2},-\frac{1}{2}} \\
\tilde{c}_{\frac{7}{2},+\frac{1}{2}}
\end{pmatrix} = \frac{1}{\sqrt{6}} \begin{pmatrix}
-\sqrt{2} - i\sqrt{2} + \sqrt{2} \\
+1 \\
+i \sqrt{3} \\
2
\end{pmatrix} \begin{pmatrix}
c_{y\uparrow} \\
c_{x\uparrow} \\
c_{x\downarrow} \\
c_{y\downarrow}
\end{pmatrix}$$

the average sign is improved due to the diagonalized hybridization function matrix $\tilde{H}$.

Results.- In Fig. 1 we plot the average sign for the four different bases considered in this work as a function of electron density (Fig. 1(a)) and spin-orbit coupling strength (Fig. 1(b,c)). The orbital-spin basis $V_{\text{os}}$ has a severe sign problem, since a drastic drop in the average sign of $V_{\text{os}}$ appears as a function of the SOC strength both below and above half-filling. Figure 2 shows the evolution of the average sign as a function of $U$ ($J_H$) at various electron fillings. The suppressed average sign of $V_{\text{os}}$ in the noninteracting limit implies that the source of the sign problem in this basis is the off-diagonal hybridization function generated by the SOC. The basis $V_{\text{eff}}$, defined in Eq. (5), diagonalizes the hybridization-function matrix of the Hamiltonian, and thus recovers the sign-free behavior in the noninteracting limit, as demonstrated in Fig. 2. In the presence of a nonzero Hund coupling $J_H$, however, $V_{\text{eff}}$ shows a sign problem as well, especially at intermediate interaction strengths and near half-filling.

In order to further improve the average sign we introduce the new basis $V_{J_{3/2BA}}$ in which $\tilde{c}_{\frac{1}{2},+\frac{1}{2}}$ and $\tilde{c}_{\frac{3}{2},-\frac{1}{2}}$ are
It turns out that $V_{\text{opt}}$ of the intra-orbital interaction strength $V$ of unity (see Fig. 2). As we show in Fig. 1(b,c), on the other hand, the difference between the average signs of $V_{j/2BA}$ and $V_{\text{eff}}$ is smaller. Since the CTHYB is based on the expansion around the localized limit, those observations imply that $V_{j/2BA}$ effectively prevents sign-problematic high-order processes.

Note that neither $V_{j/2BA}$ nor $V_{\text{eff}}$ are optimal bases for the non-SO-coupled model. As we show in Fig. 1(b,c), at the non-SO-coupled point ($\lambda = 0$), $V_{j/2BA}$ and $V_{\text{eff}}$ exhibit a sign problem in contrast to $V_{\text{os}}$. This demonstrates that Eq. (5) includes dangerous interacting terms in the $V_{j/2BA}$ and $V_{\text{eff}}$ basis. One of these terms is the correlated-hopping (CH) term, which has the form

$$\frac{\sqrt{2}J_H}{3} \sum_{s=\pm} \left[ s(2\tilde{n}_{\frac{1}{2}} - \tilde{n}_{\frac{1}{2}}) \tilde{c}_{\frac{1}{2}+\frac{1}{2}}^\dagger \tilde{c}_{\frac{3}{2}+\frac{1}{2}} + h.c. \right]$$

in $V_{\text{eff}}$, and

$$\frac{\sqrt{2}J_H}{6} \sum_{s=\pm} \left[ s(\tilde{n}_{\frac{1}{2}} - \tilde{n}_{\frac{1}{2}}) \tilde{c}_{\frac{1}{2}+\frac{1}{2}}^\dagger \tilde{c}_{\frac{3}{2}+\frac{1}{2}} + h.c. \right]$$

in $V_{j/2BA}$. This CH term is the major source of the sign problem in the SO-coupled Hamiltonian. Table I analyzes the effect of different terms in the local Hamiltonian on the average sign, for both $V_{j/2BA}$ and $V_{\text{eff}}$. There is a substantial drop in the average sign when the CH terms are introduced.

In $V_{j/2BA}$ and $V_{\text{eff}}$, there emerge other new terms involving four different flavors, which are not of the spin-flip-type or pair-hopping-type appearing in the Slater-Kanamori Hamiltonian in $V_{\text{os}}$. Those terms are denoted as four-scattering terms in Table I. The average sign in both $V_{j/2BA}$ and $V_{\text{eff}}$ becomes even lower when the CH term is combined with the pair-hopping and the four-scattering terms. In the Supplementary Material [51], we analyze the nature of the self-consistent solutions for the Hamiltonians without the CH or FS terms and we discuss the potential use of such masked Hamiltonians.

In what follows we will determine by the SPSA method the optimal basis in terms of average sign for the paramagnetic regime with the most severe sign problem and show that this optimal basis is nearly identical to the $V_{j/2BA}$ basis. For that, we search the basis space generated by the $SO(4)$ rotation group for $j = 3/2$, whose $4 \times 4$ matrix representation is denoted by $\mathbf{M}$ and transforms the electron...
operators in $V_{\text{eff}}$ as follows:

$$
\hat{a}_{\frac{3}{2}} = M \cdot \hat{c}_{\frac{1}{2}}, \quad (9)
$$

$$
\hat{a}_{\frac{1}{2}}^\dagger = \left( \hat{a}_{\frac{3}{2}}, \hat{a}_{\frac{1}{2}}, \hat{a}_{\frac{1}{2}}, \hat{a}_{\frac{1}{2}} \right), \quad (10)
$$

$$
\hat{c}_{\frac{1}{2}}^\dagger = \left( \hat{c}_{\frac{1}{2}}, \hat{c}_{\frac{1}{2}}^\dagger, \hat{c}_{\frac{1}{2}}^\dagger, \hat{c}_{\frac{1}{2}}^\dagger \right). \quad (11)
$$

Since the off-diagonal hybridization function is a clear source of the severe sign problem as shown in the cases of $V_{\text{Uos}}$ (Figs. 3 and 2), we exclude the mixing between the $j = 1/2$ and $3/2$ subspaces to preserve the diagonal structure of the hybridization. Without mixing between the $j = 1/2$ and $3/2$ subspaces, one can fix the basis for the $j = 1/2$ subspace using the rotational symmetry generated by the total angular momentum operator, $J_{\text{eff}} = L_{\text{eff}} + S$ without loss of generality.

To parametrize the basis space, we introduce the isoclinic decomposition of $M$ as $M = M_L M_R$, where

$$
M_L = \begin{pmatrix}
a & -b & -c & -d \\
-b & a & -d & c \\
c & d & a & -b \\
d & -c & b & a
\end{pmatrix}, \quad M_R = \begin{pmatrix}
p & -q & -r & -s \\
q & p & s & -r \\
r & -s & p & q \\
s & r & -q & p
\end{pmatrix}. \quad (12)
$$

Here, $a^2 + b^2 + c^2 + d^2 = 1$ and $p^2 + q^2 + r^2 + s^2 = 1$.

FIG. 3. (a) Average sign of the positively and negatively perturbed parameter points during the SPSA search for the $SO(4)$ group ($n = 3.5$, $T = 0.03$, $\lambda = 0.25$, $U = 2.0$, and $J_{\text{H}}/U = 0.15$) as a function of iterations. The inset shows the convergence of the parameters defined in Eqs. (12). (c) Landscape of the average sign in the $(\theta_1, \theta_2)$ subspace described by Eq. (13). Green triangles represent the SPSA trajectory of (c). The numeric labels in (b) denote iteration numbers during the SPSA search and the arrow in (c) shows the direction in which the search proceeds.

Under these constraints among $\{a, b, c, d\}$ and $\{p, q, r, s\}$ the dimension of the parameter space becomes 6.

Figure 3 shows how the SPSA works while searching for the optimal basis in this parameter space. The evolution of the average sign as a function of number of iterations at both positively (sign$^+$) and negatively (sign$^-$) perturbed points in the parameter space are shown in Fig. 3(a). The average sign value converges to $\sim 0.74$ for $n = 3.5$, $T = 0.03$, $\lambda = 0.25$, $U = 2.0$, and $J_{\text{H}}/U = 0.15$. Within numerical accuracy, it is very close to the value of $V_{3/2BA}$ defined in Eq. (13). This shows that the $V_{3/2BA}$ basis is at least near the local optimum in parameter space. The insets of Fig. 3(a) illustrate the convergence of the parameters in Eqs. (12).

Figure 3(b,c) show the SPSA sequence in a small parameter subspace. We introduce two parameters $\theta_1$ and $\theta_2$ representing the restricted basis transformation

$$
M = \begin{pmatrix}
cos \theta_1 & \sin \theta_1 & 0 & 0 \\
-\sin \theta_1 & \cos \theta_1 & 0 & 0 \\
0 & 0 & \cos \theta_2 & \sin \theta_2 \\
0 & 0 & -\sin \theta_2 & \cos \theta_2
\end{pmatrix}. \quad (13)
$$

Figure 3(c) shows that the landscape of the average sign is smooth, so that the SPSA search based on the gradient approximation can successfully find the local optimum in that subspace. Furthermore, $V_{3/2BA}$, corresponding to $\theta_1 = 0$ and $\theta_2 = \pi/4$, is shown to be very close to the optimum found by the SPSA. Figure 3(b) plots the trajectory determined by the SPSA.

We finally investigate the temperature scaling of the average sign for the different bases. Figure 4 shows the exponential scaling (sign) $\sim \exp(-\beta \delta F + F_0)$ as a function of inverse of temperature $\beta$. Here, $\delta F$ can be regarded as the free-energy difference from the auxiliary
bosonic system without sign problem, which determines the temperature scaling. For both fillings, \( n = 3.5 \) and 2.5, the \( V_{3/2BA} \) basis shows an improved temperature scaling exponent \( \delta F \) and a comparable offset \( F_0 \).

Conclusion.- We have investigated the nature of the sign problem in the CTHYB for the SO-coupled multi-orbital Hubbard model. We found that the correlated hopping term that appears in the \( j_{\alpha \beta} \) basis is the major source of the sign problem, and we suggest a new basis –the \( j = 3/2 \) bonding-antibonding basis– which alleviates the effects of those terms. By applying the stochastic optimization scheme, we found that the \( j = 3/2 \) bonding-antibonding basis is near a local optimum in our parameter space. With these results (i) we provide a useful guideline for the choice of the single-particle basis in CTHYB simulations of SO-coupled systems, and (ii) we propose an algorithm to numerically determine the optimal basis.

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[54] See Supplemental Material at [URL will be inserted by publisher] for data of self-consistent solution of the masked Hamiltonians.
Supplemental Information: Alleviating the Sign Problem in Quantum Monte Carlo Simulations of Spin-Orbit-Coupled Multi-orbital Hubbard Models

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I. Self-consistent solution of the masked Hamiltonians

In this section, we investigate the nature of the self-consistent solutions for masked Hamiltonians. Since we can increase the average sign substantially by dropping the most problematic correlated hopping (CH) or four-scattering (FS) terms, those masked Hamiltonians potentially provide a useful approximation of the full Hamiltonian if the self-consistent solution is sufficiently close the one for the full Hamiltonian.

The masking of those terms, however, modifies the local eigenstates. Table SI shows the form of the ground states of the full local Hamiltonian in $V_{\text{eff}}$ defined in the main text. When we mask the CH or FS terms, the ground state degeneracy of the full local Hamiltonian is broken in the $N = 2$ and $3$ sectors. Table SII and SIII present the ground states for the masked local Hamiltonians without the CH and FS term, respectively. The remaining ground states for the $N = 2$ and $3$ sectors depend on the type of masked terms. When the FS terms are dropped, the form of the highest $|J_z|$ ground state remains the same as for the full Hamiltonian. Since the FS terms involve four different flavors by definition, they become irrelevant for the highest $|J_z|$ states with fixed $j = 3/2$ and $m_j = \pm 3/2$ electrons. On the other hand, masking the CH terms selects the $|J_z| = 1$ states for the $N = 2$ sector and the $|J_z| = 1/2$ states for the $N = 3$ sector with slightly modified coefficients, which demonstrates the relevance of these terms for the highest $|J_z|$ states.

Such a modified degeneracy of the local Hamiltonian leads to substantial changes in observables especially when the system becomes localized. In Fig. S1(a,c,e), for example, one can see a sizable difference between the electron densities from the full and masked local Hamiltonians for the large-$U$ Mott insulator. The degeneracy of the electron density between the $j = 3/2$, $m_j = \pm 1/2$ and $m_j = \pm 3/2$ flavors is naturally broken for the masked Hamiltonian. Mott localization is signaled by the suppression of the spectral function at the Fermi-level, and this quantity can be approximately evaluated as $A(\omega = 0) = -\frac{1}{\pi T}G(\tau = \beta/2)$ . Moreover the Mott transition point $U_{\text{c}}$ for $n = 2$ and 4 is reduced as we mask the CH or FS terms. Compared to the FS-dropped Hamiltonian, the CH-dropped one shows a further reduction in $U_{\text{c}}$ for the $n = 2$ case. This kind of $U_{\text{c}}$ reduction as a result of a degeneracy breaking has been reported in non-spin-orbit-coupled system in the presence of a single-particle crystal-field splitting, and in the absence of the spin-flip and pair-hopping terms, (so-called Ising-type Hund coupling) at the many-body level (See Fig. S2).

One interesting observation is that the density values of the full Hamiltonian are approximately recovered by the masked one if we artificially symmetrize the $j = 3/2$, $m_j = \pm 1/2$ and $m_j = \pm 3/2$ flavors during the self-consistency loop of the DMFT. Figure S3 shows the corresponding electron density and the approximated spectral function at the Fermi level. The density values become much closer to those of the full Hamiltonian. Especially, the FS-dropped Hamiltonian at and below half-filling yields results which are consistent within $\sim 5\%$ relative error. As a result of the modification of the Hamiltonian, the sign problem of the CTHYB simulation is alleviated by up to $\sim 15\%$. When applied with proper care, this symmetrization trick could provide a useful estimate for physical observables when the original Hamiltonian cannot be treated due to the serious sign problem.

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2 L. Huang, L. Du, and X. Dai, Phys. Rev. B 86, 035150 (2012).
Figure S1: Electron density (upper panels) and approximate spectral function at the Fermi-level (lower panels) as a function of interaction strength $U$ for various total electron fillings. Both observables are measured from the self-consistent solutions of the full and masked Hamiltonians. For the masked Hamiltonians, the FS and CH terms are dropped in the $V_{\text{Jeff}}$, respectively.

Figure S2: Approximate spectral function at the Fermi-level for the non-spin-orbit-coupled three-orbital system with Ising-type Hund coupling. Compared to the rotationally-invariant Hund coupling, the Mott transition point $U_c$ is suppressed by $\sim 10\%$ for $n = 2$, $T = 1/30$ and $J_H = 0.15U$.

Figure S3: Electron density (upper panels) and the approximate spectral function at the Fermi-level (lower panels) as a function of interaction strength $U$ for various total electron fillings. Both observables are measured from the symmetrized self-consistent solutions of the full and masked Hamiltonians. The symmetrization between the $j = 3/2$, $m_j = \pm 1/2$ and $m_j = \pm 3/2$ Green functions is done at every DMFT iteration step. For the masked Hamiltonians, the FS and CH terms are dropped in the $V_{\text{Jeff}}$ basis, respectively.
Table SII: Ground state for a given sector of the full local Hamiltonian. In our notation, the upper (lower) level represents the $j = 1/2$ (3/2) flavors and the lower left (right) level corresponds to the $m_j = \pm 1/2$ ($m_j = \pm 3/2$) flavor. Full (empty) circles mark the positive (negative) $m_j$ electron. The subscript of the coefficients represents the corresponding $N$ sector.

| $N$ | $J_z$ | Ground State |
|-----|-------|--------------|
| 2   | +1    | $\alpha_2'$ $\alpha_2$ $\alpha_2$ $\alpha_2$ |
| 2   | -1    | $\alpha_2''$ $\alpha_2''$ $\alpha_2''$ $\alpha_2''$ |
| 3   | +1/2  | $\alpha_3'$ $\alpha_3'$ $\alpha_3'$ $\alpha_3'$ |
| 3   | -1/2  | $\alpha_3''$ $\alpha_3''$ $\alpha_3''$ $\alpha_3''$ |
| 4   | 0     | $\alpha_4$ $\alpha_4$ $\alpha_4$ $\alpha_4$ |

Table SII: Ground state for a given sector of the local Hamiltonian without the correlated-hopping terms. In our notation, the upper (lower) level represents the $j = 1/2$ (3/2) flavors and the lower left (right) level corresponds to the $m_j = \pm 1/2$ ($m_j = \pm 3/2$) flavor. Full (empty) circles mark the positive (negative) $m_j$ electron.

| $N$ | $J_z$ | Ground State |
|-----|-------|--------------|
| 2   | +1    | $\alpha_2''$ $\alpha_2''$ $\alpha_2''$ $\alpha_2''$ |
| 2   | -1    | $\alpha_2''$ $\alpha_2''$ $\alpha_2''$ $\alpha_2''$ |
| 3   | +1/2  | $\alpha_3''$ $\alpha_3''$ $\alpha_3''$ $\alpha_3''$ |
| 3   | -1/2  | $\alpha_3''$ $\alpha_3''$ $\alpha_3''$ $\alpha_3''$ |
| 4   | 0     | $\alpha_4'$ $\alpha_4'$ $\alpha_4'$ $\alpha_4'$ |

Table SIII: Ground state for a given sector of the local Hamiltonian without the four-scattering terms. In our notation, the upper (lower) level represents the $j = 1/2$ (3/2) flavors and the lower left (right) level corresponds to the $m_j = \pm 1/2$ ($m_j = \pm 3/2$) flavor. Full (empty) circles mark the positive (negative) $m_j$ electron.

| $N$ | $J_z$ | Ground State |
|-----|-------|--------------|
| 2   | +2    | $\alpha_2$ $\alpha_2$ $\alpha_2$ $\alpha_2$ |
| 2   | -2    | $\alpha_2$ $\alpha_2$ $\alpha_2$ $\alpha_2$ |
| 3   | +3/2  | $\alpha_3'$ $\alpha_3'$ $\alpha_3'$ $\alpha_3'$ |
| 3   | -3/2  | $\alpha_3'$ $\alpha_3'$ $\alpha_3'$ $\alpha_3'$ |
| 4   | 0     | $\alpha_4'$ $\alpha_4'$ $\alpha_4'$ $\alpha_4'$ |