Symmetries and Canonical Transformations of the Hubbard Model on Bipartite Lattices

Stellan Östlund
Institute of Theoretical Physics, Chalmers University of Technology, S-41296, Göteborg, Sweden
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Recently an exact SU(2)⊗SU(2) symmetry for the half-filled Hubbard model has been elucidated but has not yet been properly incorporated in many analyses of this model. We compute the irreducible representations of the symmetry group, a necessary step for any consistent mean-field analysis. A proper mean-field theory valid for both negative- and positive-U Hubbard models is then presented. A by-product of the description is a systematic enumeration of the Lie group SU(8) of unitary canonical transformations that is a direct generalization of the SU(4) transformation in the theory of superfluid ^{3}He and the SU(2) Bogoliubov transformation in BCS theory.

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In spite of the fact that the Hubbard model has served as a paradigm for strongly correlated electrons on a lattice, only recently has it been appreciated that in addition to the ordinary SU(2) spin symmetry, there exists an exact "hidden" SU(2) "pseudospin" symmetry at half filling [1–3]. The existence of the hidden symmetry calls into question the calculations that have been done in the past on the Hubbard model, since the order parameters that have been considered have *not* been shown to be representations for the full symmetry group. This is a minimal requirement for a self-consistent mean-field or long-wavelength theory. Deficiencies in previous mean-field theories are further suggested by the fact that these calculations have been able to treat both the attractive and repulsive Hubbard model at the same time.

We remedy this by providing a systematic analysis of order parameters of the SU(2)⊗SU(2) symmetry of the Hubbard model at half filling and show that this group forms a natural subgroup of an SU(4) symmetry of the noninteracting theory. The classifications of the representations of the full symmetry group are relevant for *any* type of analysis of the half-filled Hubbard model. In this paper we perform a mean-field analysis which can be seen to be a natural extension of Hartree-Fock and BCS theory. But here, since the action of the symmetry group turns out to mix Hartree-Fock and "BCS" expectation values, a self-consistent theory is possible only by taking into account the possibility of nonzero expectation values of *all* quadratic forms of creation and annihilation operators. A by-product of our description is a natural extension of the theory of superfluid ^{3}He to a system with the possibility of three broken symmetries: electromagnetic gauge, spin, and odd-even sublattice.

The Hubbard model at half filling is given by the Hamiltonian [4]

$$H = H_0 + U \sum_r S(r)^2 , \tag{1}$$

where $S(r) = \sum_{\alpha\beta} c^\dagger_{\alpha,r} \sigma_{\alpha,\beta} c_{\beta,r}$ and σ is the vector of Pauli matrices. The Hamiltonian H_0 is given by the usual tight-binding hopping $H_0 = -t\sum c^\dagger_{\sigma,r} c_{\sigma,r'}$, where the summation is over spin σ and grid points r and nearest neighbors r' of an arbitrary dimensional cubic lattice. The creation operator of an electron with spin σ at site r is labeled $c^\dagger_{\sigma,r}$.

The Hamiltonian H_0 is diagonalized as $H_0 = \sum_{k\alpha} \epsilon^0_k c^\dagger_{\sigma,k} c_{\sigma,k}$. The sum on k runs from $-\pi$ to π for each k_j, and the single particle energy is given by $\epsilon^0_k = -2t\sum_j \cos k_j$, where k_j denotes each component of the vector k.

We define the vector $Q = (\pi, \ldots, \pi)$ and the operators

$$\begin{aligned} a^\dagger_k &\equiv (a^\dagger_{\uparrow,k}, a^\dagger_{\downarrow,k}) = (c^\dagger_{\uparrow,k}, c^\dagger_{\downarrow,k}), \quad \text{when } \epsilon^0_k < 0 , \\ b^\dagger_k &\equiv (b^\dagger_{\uparrow,k}, b^\dagger_{\downarrow,k}) = (c^\dagger_{\uparrow,k+Q}, c^\dagger_{\downarrow,k+Q}), \quad \text{when } \epsilon^0_k > 0 , \end{aligned} \tag{2}$$

so that in terms of these operators

$$H_0 = \sum_{k\alpha} \epsilon^0_k (a^\dagger_{\sigma,k} a_{\sigma,k} - b^\dagger_{\sigma,k} b_{\sigma,k}) , \tag{3}$$

where now the summation runs over the reduced Brillouin zone corresponding to $\epsilon^0_k < 0$.

The "Lieb-Mattis" transformation Z acts on the *position space* creation and destruction operators $c^\dagger_{\sigma,r}$ through the canonical transformation $c^\dagger_{\downarrow r} \mapsto -1^r c_{\downarrow r}$, $c^\dagger_{\uparrow r} \mapsto c^\dagger_{\uparrow r}$, where $-1^r \equiv e^{iQ\cdot r}$. Spin rotations and Z act naturally on an 8-component multispinor of definite momentum: $\Psi_k \equiv (a_k, b_k, a^\dagger_{-k}, b^\dagger_{-k})$. In momentum space Z can be represented by the idempotent matrix whose entries are all zero except $Z_{1,1} = Z_{3,3} = Z_{5,5} = Z_{7,7} = Z_{2,8} = Z_{4,6} = Z_{6,4} = Z_{8,2} = 1$. The Lieb-Mattis transformation then becomes $\Psi_k \mapsto Z\Psi_k$. It is well known that Z is an exact symmetry of H_0 but changes the sign of the Hubbard term U [2–5].

Spin rotations are defined using eight-dimensional representations of the Dirac gamma matrices [6] in the "standard representation" where γ_0 is diagonal with entries $(1, 1, -1, -1)$. We define the seven 8×8 matrices β_A written in block form as

$$\beta_0 = \begin{pmatrix} \gamma_0 & 0 \\ 0 & -\gamma_0 \end{pmatrix}, \quad \beta_j = \begin{pmatrix} \gamma_j & 0 \\ 0 & \gamma_j^* \end{pmatrix},$$

and $\beta_{j+3} = iZ\beta_0\beta_j Z$, all for $1 \le j \le 3$. The notation γ_j^* denotes complex conjugate (*not adjoint*).

By explicit computation, it can be verified that these seven matrices β_A obey $\beta_A\beta_B + \beta_A\beta_B = 2g_{AB}$, where g_{AB} is the diagonal operator $(1,-1,-1,-1,-1,-1,-1)$ times the unit matrix. Thus β_ν defines an 8×8 Clifford algebra. The matrix β_0 obeys the constraint $\beta_0 = i\beta_1\beta_2\beta_3\beta_4\beta_5\beta_6$.

We define the commutators between the β matrices $M_{A,B} \equiv \frac{i}{2}[\beta_A, \beta_B]$. A series of corollaries now follow directly from the general relation between SO($2n$) and SO($2n+1$) and Clifford algebras of $2^n \times 2^n$ matrices [7].

$M_{A,B}$ defines the Lie algebra of SO(6,1) for $0 \le A, B \le 6$. The restriction $A, B \ne 0$ generates the subalgebra of SO(6) which is known to be isomorphic to SU(4). By construction $M_{i,j}$ for $1 \le i,j \le 3$ generates the SU(2) subalgebra of spin rotations. Since β_0 anticommutes with β_A and it can be checked that β_0 commutes with Z we find that $ZM_{i,j}Z = M_{i+3,j+3}$ so that $M_{i+3,j+3}$ generates another SU(2) subalgebra defined by the $SU(2)_P$ "pseudospin" symmetry that is known to be a symmetry of the Hubbard model, and corresponds to conjugating ordinary spin rotations with the Mattis-Lieb transformation Z. Since it anticommutes with all other β_A, the matrix β_0 is a scalar under the SO(6) defined by $M_{A,B}$ for $A, B \ne 0$.

Since the Hamiltonian H_0 is simply given in terms of β_0 by $H_0 = \frac{1}{2}\sum_k \epsilon_k^0 \Psi_k^\dagger \beta_0 \Psi_k$ we see immediately that H_0 is in fact invariant under the entire group SO(6)≈SU(4) generated by $M_{A,B}$.

To understand how this group is imbedded, we investigate a general canonical transformation of the form $\Psi_k \mapsto T_k\Psi_k$ and $\Psi_{-k} \mapsto T_{-k}\Psi_{-k}$. We define the matrix $g = -\beta_1\beta_3\beta_5 = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$ in 4×4 block form. Preservation of the canonical anticommutation relations is then equivalent to $T_k g \tilde{T}_{-k} = g$. Here the tilde indicates transpose. If we *also* impose the restriction that T_k generate a unitary transformation, we demand that $g(T_{-k})^* g = T_k$ resulting in $T_k(T_k)^\dagger = 1$ which identifies T_k as an element of U(8). Demanding a global transformation results in the additional constraint $T_k \equiv T$ for all values of k. In terms of infinitesimal generators $T_k \approx 1 + G_k$ we then have three conditions

$$\begin{aligned} &gG_k g = -\tilde{G}_{-k}, \quad \text{canonical}, \\ &gG_k g = (G_{-k})^*, \quad \text{unitary}, \\ &G_k = G\forall_k, \quad \text{global}. \end{aligned} \tag{4}$$

The entire group of unitary canonical transformations is therefore a copy of U(8) for each k in the "positive reduced Brillouin zone," defined here as the first Brillouin zone modulo the operations $k \mapsto k + (\pi, \ldots, \pi)$ and $k \mapsto -k$. This generates an SU(8) analog of the SU(2) Bogoliubov transformation of BCS theory and the SU(4) theory of ^{3}He [8]; a doubling of the degrees of freedom occurs for each nonconserved variable in the set of particle number, spin, and momentum $(\pi, \ldots, \pi)$. The subgroup of global transformations is generated by all matrices $i\beta_0, \beta_A$, and all commutators of these seven matrices defines the Lie algebra of SO(7). Direct computation shows that the group SO(6) previously identified is the largest unitary subgroup that commutes with β_0.

We have thus shown that the most general set of canonical transformations that mix particles and holes, spin and momentum $(\pi, \ldots, \pi)$ is given by the product of a copy of SU(8) for each value of k in the positive reduced Brillouin zone. Requiring commutability with H_0 breaks this down to SO(6)≈SU(4) and finally requiring commutability with the Hubbard model breaks this down to global SU(2)⊗SU(2). All these embeddings are generated by Lie subalgebras created by commutators of subsets of the Clifford algebra.

Mean-field theory is built on expectation values of the form $\langle c_{\sigma,p}^\dagger c_{\delta,q}\rangle$ and $\langle c_{\sigma,p}^\dagger c_{\delta,q}^\dagger\rangle$ but in order to construct self-consistent mean-field theories of the Hubbard model we must use irreducible representations that transform properly under SU(2)⊗SU(2), Z and if possible connects to the SO(6) symmetry of the noninteracting theory. The pseudospin symmetry mixes the Hartree, Fock, *and* BCS terms and all these must therefore be incorporated in the representations. All this can be elegantly accomplished by using the matrices β_A.

We shall use the standard SU(4) notation of labeling representations by boldface numerals that coincide with their dimensionality, and complex conjugate representations by an asterisk. For SU(4) representations **1**, **4**, **6**, **10**, and **15**, only **4** and **10** are inequivalent from their complex conjugate. We first note that Ψ_k forms an eight-dimensional reducible representation of SU(4). Since β_0 commutes with the generators $M_{A,B}$, the projection operator which decomposes the eight-dimensional representation into two 4D representations $\mathbf{4} \oplus \mathbf{4}^*$ is precisely $1 \pm \beta_0$.

In order to understand how the group acts on operators we next decompose tensor products such as $\Psi_p^\dagger \otimes \Psi_q$ into irreducible representations. These are given by [9] $\mathbf{4} \otimes \mathbf{4}^* = \mathbf{1} \oplus \mathbf{15}$ and $\mathbf{4} \otimes \mathbf{4} = \mathbf{6} \oplus \mathbf{10}$. This then yields the decomposition $\Psi_p^\dagger \otimes \Psi_q \approx (\mathbf{4} \oplus \mathbf{4}^*) \otimes (\mathbf{4}^* \oplus \mathbf{4}) = 2(\mathbf{1} \oplus \mathbf{15}) \oplus 2(\mathbf{6}) \oplus (\mathbf{10} \oplus \mathbf{10}^*)$.

When SU(4) breaks down to $SU(2)_S \otimes SU(2)_P$, these representations branch [9] according to

$$\begin{aligned} &\mathbf{4} \mapsto (D^{\frac{1}{2}} \otimes D^{\frac{1}{2}}), \\ &\mathbf{6} \mapsto (D^1 \otimes D^0) \oplus (D^0 \otimes D^1), \\ &\mathbf{10} \mapsto (D^1 \otimes D^1) \oplus (D^0 \otimes D^0), \\ &\mathbf{15} \mapsto (D^1 \otimes D^1) \oplus (D^1 \otimes D^0) \oplus (D^0 \otimes D^1), \end{aligned} \tag{5}$$

where $D^\nu \otimes D^\mu$ indicates the D^ν representation of $SU(2)_P$ and D^μ indicates the spin μ representation of $SU(2)_S$. Here subscripts P and S denote "pseudospin" and "spin," respectively.

Using this information, we see that when $\Psi_p^\dagger \otimes \Psi_q$ splits into irreducible representations of $SU(2)_P \otimes SU(2)_S$, we induce a decomposition into $4(D^0 \otimes D^0) \oplus 4(D^1 \otimes D^0) \oplus 4(D^0 \otimes D^1) \oplus 4(D^1 \otimes D^1)$.

The branching of the irreducible representations is most easily described by associating a polynomial of fermion operators with a matrix: $\mathcal{O}_{p,q}(m) \equiv \sum_{i,j} (\bar{\Psi}_p)_i m_{ij} (\Psi_q)_j$, where we have defined $\bar{\Psi}_p \equiv \Psi_p^\dagger \beta_0$. We further define the 8×8 SU(2)$\otimes$SU(2) scalar matrix Γ by

$$\Gamma = i\beta_0\beta_1\beta_2\beta_3 = \begin{pmatrix} \gamma_5 & 0 \\ 0 & \gamma_5 \end{pmatrix} ,$$

where γ_5 indicates the ordinary pseudoscalar $\gamma_5 = i\gamma_0\gamma_1\gamma_2\gamma_3$.

The coefficients linking the 8×8 matrices to each of the invariant spaces that form representations of SU(4) and of Z can then be neatly represented by products of the beta matrices. We denote the four $SU(2)_P \otimes SU(2)_S$ scalars by Υ with the following superscripts: $\Upsilon^0 = 1 - \beta_0$, $\Upsilon^{0^*} = 1 + \beta_0$, $\Upsilon^1 = (1+\beta_0)\Gamma$, $\Upsilon^{1^*} = -(1-\beta_0)\Gamma$. To make subsequent formulas simple we also need to define $\Omega_0 = \Omega^0 = \Gamma$, $\hat{\Omega}_0 = \hat{\Omega}^0 = \Gamma$, $\Omega_i = \Omega^i = \beta_i$, and $\hat{\Omega}_i = -\hat{\Omega}^i = i\beta_{i+3}$. With all these definitions, the irreducible representations can be written in the following natural "4-vector" form

$$(\Upsilon^\tau_{\mu,\nu})_{p,q} \equiv \mathcal{O}_{p,q}\,(\Upsilon^\tau\ \Omega^\mu \hat{\Omega}_\nu) \,, \qquad (\Upsilon^{\tau^*}_{\mu,\nu})_{p,q} \equiv \mathcal{O}_{p,q}\,(\Upsilon^{\tau^*}\ \hat{\Omega}_\nu \Omega^\mu) \,, \tag{6}$$

where $0 \le \mu, \nu \le 3$.

We can now classify all possible bilinear order parameters according to their irreducible representations of SU(4) and $SU(2)_S \otimes SU(2)_P$ using the following linear combinations whose relation to usual Fermi operators is suggested by their symbols. Sum over repeated indices is implied,

$$\begin{aligned} M^{ab,j}_{p,q} &= \langle a^\dagger_{\delta,p} (\sigma_j)_{\delta,\tau} b_{\tau,q} \rangle \,, \\ N^{ab}_{p,q} &= \langle a^\dagger_{\delta,p} b_{\delta,q} \rangle \,, \\ \Delta^{ab,\mu}_{p,q} &= \langle a^\dagger_{\delta,p} (i\sigma_2\sigma_\mu)_{\delta,\tau} b^\dagger_{\tau,-q} \rangle \,, \\ \Delta^{*ab,\mu}_{p,q} &= \langle a_{\delta,-p} (i\sigma_2\sigma_\mu)_{\delta,\tau} b_{\tau,q} \rangle \,, \end{aligned} \tag{7}$$

and similar definitions for $M^{aa,j}_{p,q}$, etc. We have defined σ_0 to be the identity matrix.

The different representations of SU(4) can be naturally organized into 4×4 form, where each column transforms as a 4-vector under $SU(2)_S$ and each row transforms as a 4-vector under $SU(2)_P$, i.e., the zero component transforms as a scalar, and the one-two-three component like an ordinary vector under the respective rotation group. Each irreducible representation of SU(4) is contained in exactly one of the diagrams by combining appropriate subblocks. The subblocks are easily identified by matching the dimensionality. We use the notation $(10) \equiv D^1 \otimes D^0$, etc.,

$$\langle (\Upsilon^0_{\mu\nu})_{p,q} \rangle = [\mathbf{1}]_{p,q} \oplus [\mathbf{15}]_{p,q} \mapsto [00]_{p,q} \oplus [(01) \oplus (10) \oplus (11)]_{p,q} \,, \tag{8}$$

(9)

$N^{aa}_{-q,-p} - N^{bb}_{p,q}$	$\Delta^{ab,0}_{-q,p} + \Delta^{*ba,0}_{-q,p}$	$-i\Delta^{ab,0}_{-q,p} + i\Delta^{*ba,0}_{-q,p}$	$N^{aa}_{-q,-p} + N^{bb}_{p,q} - \delta_{p,q}$
$M^{aa,x}_{-q,-p} + M^{bb,x}_{p,q}$	$\Delta^{ab,x}_{-q,p} + \Delta^{*ba,x}_{-q,p}$	$-i\Delta^{ab,x}_{-q,p} + i\Delta^{*ba,x}_{-q,p}$	$M^{aa,x}_{-q,-p} - M^{bb,x}_{p,q}$
$M^{aa,y}_{-q,-p} + M^{bb,y}_{p,q}$	$\Delta^{ab,y}_{-q,p} + \Delta^{*ba,y}_{-q,p}$	$-i\Delta^{ab,y}_{-q,p} + i\Delta^{*ba,y}_{-q,p}$	$M^{aa,y}_{-q,-p} - M^{bb,y}_{p,q}$
$M^{aa,z}_{-q,-p} + M^{bb,z}_{p,q}$	$\Delta^{ab,z}_{-q,p} + \Delta^{*ba,z}_{-q,p}$	$-i\Delta^{ab,z}_{-q,p} + i\Delta^{*ba,z}_{-q,p}$	$M^{aa,z}_{-q,-p} - M^{bb,z}_{p,q}$

$$\langle (\Upsilon^1_{\mu\nu})_{p,q} \rangle = [\mathbf{6}]_{p,q} \oplus [\mathbf{10}]_{p,q} \mapsto [(01) \oplus (10)]_{p,q} \oplus [(00) \oplus (11)]_{p,q} \,, \tag{10}$$

(11)

$-N^{ab}_{p,q} + N^{ab}_{-q,-p}$	$\Delta^{aa,0}_{p,-q} + \Delta^{*bb,0}_{-q,p}$	$-i\Delta^{aa,0}_{p,-q} + i\Delta^{*bb,0}_{-q,p}$	$N^{ab}_{p,q} + N^{ab}_{-q,-p}$
$M^{ab,x}_{p,q} + M^{ab,x}_{-q,-p}$	$-\Delta^{aa,x}_{p,-q} + \Delta^{*bb,x}_{-q,p}$	$i\Delta^{aa,x}_{p,-q} + i\Delta^{*bb,x}_{-q,p}$	$-M^{ab,x}_{p,q} + M^{ab,x}_{-q,-p}$
$M^{ab,y}_{p,q} + M^{ab,y}_{-q,-p}$	$-\Delta^{aa,y}_{p,-q} + \Delta^{*bb,y}_{-q,p}$	$i\Delta^{aa,y}_{p,-q} + i\Delta^{*bb,y}_{-q,p}$	$-M^{ab,y}_{p,q} + M^{ab,y}_{-q,-p}$
$M^{ab,z}_{p,q} + M^{ab,z}_{-q,-p}$	$-\Delta^{aa,z}_{p,-q} + \Delta^{*bb,z}_{-q,p}$	$i\Delta^{aa,z}_{p,-q} + i\Delta^{*bb,z}_{-q,p}$	$-M^{ab,z}_{p,q} + M^{ab,z}_{-q,-p}$

The other two independent blocks Υ^{τ^*} are obtained essentially by taking the Hermitian conjugate of the forms above. Phase factors are incorporated in our definition of the representation so that under the transformation Z each of the representations represented in this manner transforms to its transpose: $Z(\Upsilon^\tau_{\mu,\nu})_{p,q}Z = (\Upsilon^\tau_{\nu,\mu})_{p,q}$. Under the *adjoint operation*

$$[(\Upsilon^\tau_{\mu,\nu})_{p,q}]^\dagger = (\Upsilon^{\tau^*}_{\mu,\nu})_{-q,-p} = -g(\Upsilon^\tau_{\mu\nu})^* g \,, \tag{12}$$

$$[(\Upsilon^{\tau^*}_{\mu,\nu})_{p,q}]^\dagger = (\Upsilon^\tau_{\mu,\nu})_{-q,-p} = -g(\Upsilon^{\tau^*}_{\mu\nu})^* g \,, \tag{13}$$

where g is the tensor defined above Eq. (4).

A general mean-field theory consistent with translational invariance within a sublattice and SU(2)$\otimes$SU(2) must obey $(\Upsilon^\tau_{n,n'})_{p,q} = 0$ unless $p \neq q$. We must then consider the possibility of nonzero expectation values of bilinears of the form $\langle (\Upsilon^\tau_{\mu,\nu})_{k,k} \rangle$. To simplify subsequent formulas, we define the operators $(\Upsilon^\pm_{\mu,\nu})_{p,q} = \frac{1}{2}[(\Upsilon^1_{\mu,\nu})_{p,q} \pm (\Upsilon^{1*}_{\mu,\nu})_{p,q}]$ and define the order parameters

$$\overline{\Upsilon}^\tau_{0,n'} = \sum_q \langle (\Upsilon^\tau_{0,n'})_{q,q} \rangle \,. \tag{14}$$

We then take all possible nonvanishing terms of this form in the Hubbard potential and find that after considerable calculation the effective interaction is given by

$$U\sum_{p}[\overline{\Upsilon}^{+}_{0,n'}(\Upsilon^{+}_{0,n'})_{p,p}-\overline{\Upsilon}^{+}_{n,0}(\Upsilon^{+}_{n,0})_{p,p}] + [\overline{\Upsilon}^{0}_{0,n'}(\Upsilon^{0}_{0,n'})_{p,p}-\overline{\Upsilon}^{0}_{n,0}(\Upsilon^{0}_{n,0})_{p,p}]\ , \quad (15)$$

where repeated indices are summed over. Since $\Upsilon^{\tau}_{\mu,\nu}$ is transposed under Z, we see that the interaction is indeed odd under changing the sign of U, and the mean-field theory behaves properly under SU(4), Z, and the entire group SU(2)⊗SU(2).

We identify $\Upsilon^{\tau}_{n,0}$ as the order parameters that measure spontaneously broken $\mathrm{SU}(2)_S$ symmetry. The order parameters that measure broken $\mathrm{SU}(2)_P$ symmetry are $\Upsilon^{\tau}_{0,n'}$. To understand these we convert $\overline{\Upsilon}^{\tau}_{n,n'}$ to real space and define $\Delta^0_r \equiv \langle c^{\dagger}_{\uparrow,r}c^{\dagger}_{\downarrow,r}\rangle$. We find that

$$\begin{aligned}
\overline{\Upsilon}^{0}_{0,n'} &= \sum_r[-1^r\mathrm{Re}\Delta^0_r,\ -1^r\mathrm{Im}\Delta^0_r,\ (n_r-1)]\ ,\\
\overline{\Upsilon}^{0}_{n,0} &= \sum_r(M^x_r,\ M^y_r,\ M^z_r)\ ,\\
\overline{\Upsilon}^{+}_{0,n'} &= \sum_r[\mathrm{Re}\Delta^0_r,\ \mathrm{Im}\Delta^0_r,\ -1^r(n_r-1)]\ ,\\
\overline{\Upsilon}^{+}_{n,0} &= \sum_r(-1^rM^x_r,\ -1^rM^y_r,\ -1^rM^z_r)\ .
\end{aligned} \quad (16)$$

To work further with the mean-field theory, we can fix a value in $\mathrm{SU}(2)_S\otimes\mathrm{SU}(2)_P$ parameter space to determine the direction of spontaneously broken symmetry, and thereby, without loss of generality, choose

$$0=\overline{\Upsilon}^{\tau}_{0,1}=\overline{\Upsilon}^{\tau}_{0,2}=\overline{\Upsilon}^{\tau}_{1,0}=\overline{\Upsilon}^{\tau}_{2,0} \quad (17)$$

as an additional condition which resolves the ground-state $\mathrm{SU}(2)_S\otimes\mathrm{SU}(2)_P$ degeneracy.

We see that by restricting ourselves to Eq. (17) we are permitting to be nonzero precisely those expectation values that transform as the z component of spin and pseudospin. Rotations about the pseudospin z is the subgroup U(1) of electromagnetic gauge transformations. Our choice of $\mathrm{SU}(2)_P$ parametrization and broken symmetry axis selects exactly those ground states that have definite particle number, and leads to the standard "Hartree-Fock" results for the Hubbard model that define the z axis to be the axis of broken $\mathrm{SU}(2)_S$ symmetry (see for instance Ref. [4]).

Results from that analysis are unambiguous for a repulsive Hubbard model with $U>0$. Making use of standard results we obtain a Néel ordered ground state, i.e., all $\overline{\Upsilon}^{\tau}_{\mu,\nu}=0$ except $\overline{\Upsilon}^{+}_{3,0}\neq 0$.

Since we have constructed the order parameters to transform simply under the Lieb-Mattis transformation, we find a ground state for $U<0$ with all $\overline{\Upsilon}^{\tau}_{\mu,\nu}=0$ except $\overline{\Upsilon}^{+}_{0,3}$, i.e., a charge-density wave which is analogous to Néel order along the z axis. However, since the pseudospin axis can be arbitrarily chosen, long-wavelength excitations above the mean-field ground state of the half-filled negative-U Hubbard model mixes charge-density wave and the s-wave superconducting order parameter [10]. This is the analog of the antiferromagnetic spin-density waves in the repulsive Hubbard model. A consequence of this analysis is that a mean-field calculation that searches for s-wave pairing in the $U<0$ Hubbard model will find the same ground-state energy as a mean-field analysis assuming only a charge-density wave. However, the full theory is necessary to understand the Goldstone modes that in the negative-U Hubbard model mix s-wave pairing and charge-density waves.

To summarize, we have systematically enumerated the representations of the important symmetries of noninteracting electrons on a lattice and shown how the representations branch when the symmetry of the free theory is broken by the Hubbard term. A tangible consequence has been a careful validation of the standard mean-field theory of the positive-U Hubbard model, and calculation of the analogous Goldstone modes for negative U. We can of course "quickly" derive these modes by transforming each component of the Néel order parameter with the Lieb-Mattis transformation [10], but the present analysis shows that indeed no other nonzero order parameters have been neglected in that argument.

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