Symmetry classification of bond order parameters in cuprates

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We study bond-order parameters for generalized t-J models on a square lattice. Using the plane-wave limit the considered order parameters form basis functions for irreducible representations of the symmetry transformations of the point group and of time reversal. We show that for instability wave vectors along the diagonals all possible basis functions are complex, break time reversal symmetry and thus describe flux states. For instability wave vectors along the crystalline axes, corresponding to the observed case in underdoped cuprates, there are only three representations with $A_1$, $B_1$, and $E$ symmetry which do not break time reversal symmetry. We suggest that one of them has recently been observed in resonant elastic X-ray scattering.

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There is growing evidence from nuclear magnetic resonance [1], resonant X-ray scattering and diffraction [2–8] and scanning tunneling microscopy [8–10] that charge ordered states play an important role in underdoped cuprates. In particular, a charge-modulated state with 4 incommensurate wave vectors along the crystalline axes was detected in YBCO and in Bi-based single and double layer compounds. Resonant elastic X-ray scattering showed that the charge order emerges just below the opening of the pseudogap [11] in underdoped Bi2201 [9]. The formation of the pseudogap, Fermi pockets, the appearance of quantum oscillations [12] and of charge order may thus be intimately related in these systems. It is the aim of this Letter to characterize charge ordered states in strongly interacting systems without regress to weak-coupling assumptions. Furthermore, the implications of point group and time inversion symmetries for the order parameter (OP) are more carefully taken into account than in previous treatments.

The microscopic form of the charge OP in cuprates is not clear at present. To illustrate this let us consider the following model Hamiltonian for electrons on a square lattice which generally is believed to be relevant for cuprates [13].

$$\begin{align*}
H &= -\sum_{i,j,\alpha} t_{ij} c_{i\alpha}^\dagger c_{j\alpha} + \frac{J}{4} \sum_{i,j,\alpha,\beta} c_{i\alpha}^\dagger c_{i\beta} c_{j\beta}^\dagger c_{j\alpha} + V \sum_{i,j,\alpha,\beta} c_{i\alpha}^\dagger c_{i\alpha} c_{j\beta}^\dagger c_{j\beta} + \mathbf{H},
\end{align*}$$

where $t_{ij}$ denotes the hopping amplitude of electrons between the lattice site $i$ and $j$. The second and third terms in Eq. (1) describe antiferromagnetic and Coulomb interactions between electrons on neighboring sites $i$ and $j$ with coupling constants $J$ and $V$, respectively. If double occupancies of sites are excluded Eq. (1) represents the well-known t-J model for $V = -J/2$. If the constraint of no double occupancies is enforced only globally the t-J model assumes the form of Eq. (1) with renormalized coupling constants and usual fermionic creation and annihilation operators $c_{i\alpha}^\dagger$ and $c_{i\alpha}$ for electrons on site $i$ and spin direction $\alpha$.

The interaction terms in Eq. (1) give rise to two kinds of charge OPs. A Hartree-like contraction of the third term yields an OP proportional to $\sum_{\alpha} \langle c_{i\alpha}^\dagger c_{i\alpha} \rangle$ describing the charge on the site $i$. It may vary from site to site and represents a conventional charge density wave (CDW) state. The exchange contractions of the second and third term in Eq. (1) yield an OP proportional to $\sum_{\alpha} \langle c_{i\alpha}^\dagger c_{j\alpha} \rangle$, where $i$ and $j$ are nearest neighbor sites. This state may be called a nonlocal CDW or a bond-order wave (BOW) state [14] where the CDW acquires an internal degree of freedom because the electron and hole occupy different sites. It has been shown that in the large N limit of the t-J model (which corresponds to enforcing the constraint of no double occupancies of sites only globally) the phase diagram consists in the underdoped regime of incommensurate BOW states (at zero doping of the staggered flux phase [15] as a special case) [16, 17]. At the same time the conventional CDW OP is zero showing that both kinds of charge order are independent from each other. More recently the BOW state has been studied theoretically in more detail [18–21]. Also models with more than one band [22] or more complex OPs [23] have been considered. Recently a microscopic form for the OP in underdoped YBCO and Bi2201 was proposed [8] based on experimental data from resonant X-ray scattering.

Below we classify possible OPs for BOW states by exploiting point-group and time reversal symmetries. According to general considerations [24] possible OPs must form basis functions for irreducible representations of these symmetries, barring accidental degeneracies, additional instabilities or induced higher harmonics. This general principle also applies to our case with several degenerate instability vectors at the transition point $T_c$ [25]. Using this guidance we determine all possible OPs for a BOW state with four wave vectors of the form $(\pm q, \pm q)$ and the form $(\pm q, 0)$ and $(0, \pm q)$. Since these results de-
pend only on symmetry arguments they apply in particular to strongly correlated models such as the $t$-$J$ model.

From Eq. (1) follows that the BOW OP has the form of a coupling constant times the matrix element $\langle c_{i}^\dagger c_{j} \rangle$, where $i$ and $j$ are nearest neighbors and the spin index has been dropped. To simplify the nomenclature we will call the modulated part of $\langle c_{i}^\dagger c_{j} \rangle$ OP in the following. After a Fourier transform we obtain,

$$\langle c_{i}^\dagger c_{j} \rangle = \sum_{k,q} \langle c_{k+q}^\dagger c_{k} \rangle e^{-i(q\cdot r_{i}-r_{j})\cdot k}.$$  \hspace{1cm} (2)

$r_{i}$ is the vector from the origin to the lattice site $i$. In general, the sum over $q$ in Eq. (2) will extend in the plane-wave limit only over the wave vectors corresponding to a charge instability of the normal state. They form a star of wave vectors $\{q\}$. Writing $r_{j} = r_{i} + e_{j}$, keeping $e_{j}$ fixed and performing a Fourier transformation with respect to $r_{i}$ we get

$$\sum_{r_{i}} \langle c_{i}^\dagger c_{j} \rangle e^{iq\cdot r_{i}} = \sum_{k,q} \langle c_{k+q}^\dagger c_{k} \rangle e^{i(q\cdot e_{j})\cdot k} = F(q,e_{j}).$$ \hspace{1cm} (3)

The functions $F(q,e_{j})$ are defined by Eq. (3) and represent our set of order parameters. If Umklapp terms are included the sum over $q$ may not only include primary instability vectors of the normal state but higher harmonics with wave vectors $\sum n_{l}q_{l}$ where $n_{l}$ is an integer. They form new stars and cause deviations from the plane-wave limit of the OP. Because these higher harmonics are important only near the transition to the commensurate phase we will neglect them in the following and restrict ourselves to the plane-wave limit.

The symmetry group of the square lattice is $C_{4v}$. Using the notation of Ref. 24 let us denote one of the 8 symmetry transformations by $R$. Its action on the order parameter in Eq. (3) can be written as

$$\langle c_{R^{-1}r_{i}}^\dagger c_{R^{-1}r_{j}} \rangle = \sum_{k,l} \langle c_{k+R^{-1}q}^\dagger c_{k} \rangle e^{-i(q\cdot r_{i}-r_{j})\cdot k} e^{i(k\cdot R^{-1}e_{j})},$$ \hspace{1cm} (4)

where $R$ is the 2x2 matrix representing $R$ in the two-dimensional direct space. After a Fourier transformation with respect to $r_{i}$ we find that $F(q,e_{j})$ transforms under $R$ into $F(R^{-1}q,R^{-1}e_{j})$, where $R^{-1}q$ and $R^{-1}e_{j}$ belong to the star of wave vectors and nearest neighbor bonds, respectively. This means that the set of functions $\{F(q,e_{j})\}$ forms basis functions for a (reducible) representation of $C_{4v}$. Decomposing the above reducible representation into irreducible parts the basis function of one of the irreducible representations describes the OP of the state corresponding to the global minimum of the free energy. One important feature is that in general both $q_{l}$ and $e_{j}$ are transformed under $R$ at the same time and not independently from each other. This is a crucial point in our approach.

### Table 1. Coefficients $c_{\gamma l}$

| $\gamma$ | $F_{1}$ | $F_{2}$ | $F_{3}$ | $F_{4}$ | $F_{5}$ | $F_{6}$ | $F_{7}$ | $F_{8}$ |
|----------|---------|---------|---------|---------|---------|---------|---------|---------|
| $A_{1}$  | 1       | 1       | 1       | 1       | 1       | 1       | 1       | 1       |
| $A_{2}$  | 1       | 1       | 1       | 1       | -1      | -1      | -1      | -1      |
| $B_{1}$  | 1       | -1      | 1       | -1      | 1       | 1       | -1      | -1      |
| $B_{2}$  | 1       | -1      | 1       | -1      | 1       | 1       | -1      | -1      |
| $E^{(1)}(1)$ | 1       | -1      | 1       | -1      | -1      | -1      | 1       | 1       |
| $E^{(1)}(2)$ | 1       | -1      | -1      | -1      | 1       | 1       | 1       | 1       |
| $E^{(2)}(1)$ | 1       | 1       | -1      | -1      | 1       | 1       | 1       | 1       |
| $E^{(2)}(2)$ | 1       | 1       | -1      | -1      | -1      | -1      | 1       | 1       |

A further general property of the functions $\{F(q_{l},e_{j})\}$ is related to time reversal ($T$). Denoting the corresponding operator by $T$ we get

$$TF(q_{l},e_{j}) = F^{\ast}(q_{l},e_{j}) = \sum_{k} \langle c_{k-q_{l}}^\dagger c_{k} \rangle e^{-i(q_{l}-q_{j})\cdot k},$$ \hspace{1cm} (5)

where $C_{2}$ denotes the rotation by $\pi$ and the star at $F$ the conjugate complex.

In the following we will first consider the case with 4 wave vectors along the diagonals, i.e., $q_{1} = (q,q), q_{2} = (-q,q), q_{3} = (-q,-q), q_{4} = (q,-q)$, where $q$ lies between 0 and $\pi$. The four bond directions are denoted by $e_{1} = (1,0), e_{2} = (0,1), e_{3} = (-1,0), e_{4} = (0,-1)$. It is easy to see that the following 8 functions $F_{l} = F(q_{l},e_{l}), l = 1, ..., 4$, $F_{5} = F(q_{4},e_{1}), F_{6} = F(q_{2},e_{3}), F_{7} = F(q_{1},e_{2})$, and $F_{8} = F(q_{3},e_{4})$ yield a reducible representation of $C_{4v}$. Let us denote the linear combinations of the $F_{l}$ which form basis functions for the corresponding irreducible representations $\gamma$ by

$$F(\gamma) = \sum_{l=1}^{8} c_{\gamma l} F_{l}.$$ \hspace{1cm} (6)

For the one-dimensional representations $\gamma = A_{1}, A_{2}, B_{1}, B_{2}$ one can easily determine the coefficients $c_{\gamma l}$ from the character table of $C_{4v}$. One finds that each of these representations occurs exactly once, the corresponding $c_{\gamma l}$ are given in the first 4 lines of Table 1. Using again the character table one finds that the remaining 4 functions form 2 two-dimensional representations $E^{(1)}$ and $E^{(2)}$. The corresponding $c_{\gamma l}$ are given in the lines 5-8 in Table 1.

Going back to Eq. (5) we note that for the functions $F_{l}, l = 1, ..., 8$ the phase factor $e^{i(q_{l},e_{j})} \cdot q_{l}$ is always equal to $q$. Multiplying Eq. (5) by $c_{\gamma l}$ and summing over $l$ we obtain

$$F^{\ast}(\gamma) = e^{iq_{l}C_{2}} F(\gamma).$$ \hspace{1cm} (7)

From the character table of $D_{4}$ follows that $C_{2} F(\gamma)$ is equal to $F(\gamma)$ for $\gamma = A_{1}, A_{2}, B_{1}, B_{2}$ and equal to $-F(\gamma)$ for $\gamma = E$. Combining both cases we have

$$F^{\ast}(\gamma) = \pm e^{iq} F(\gamma),$$ \hspace{1cm} (8)
where the upper sign refers to $\gamma = A_1, A_2, B_1, B_2$ and the lower sign to $\gamma = E$, respectively. As a consequence $F$ is for $q \neq 0, \pi$ neither real nor imaginary but necessarily complex. Splitting Eq. (8) into real and imaginary parts yields two homogeneous equations with a vanishing determinant. Expressing then the imaginary by the real part one gets,

$$F(\gamma) = \left(1 + i\frac{\cos q - 1}{\sin q}\right)\text{Re}F(\gamma).$$  \hspace{1cm} (9)

This equation demonstrates that both the real and the imaginary part of $F(\gamma)$ can serve as basis functions for the representation $\gamma$. Including $T$ in the representation requires the above ratio of real and imaginary parts of $F(\gamma)$.

For $q = 0$ or $\pi$ the four functions $F_1, \ldots, F_4$ with $q_l = 0$ form a basis for a reducible representation of $C_{4\pi}$ which decomposes into $A_1, B_1$ and $E$ representations with the basis functions $F_1 + F_2 + F_3 + F_4, F_1 - F_2 + F_3 - F_4$ and $F_1 - F_3, F_2 - F_4$, respectively. Since $\gamma$ still holds the first two basis functions are real (imaginary) and the third and fourth ones imaginary (real) for $q = 0$ ($q = \pi$).

Included as a special case is the staggered flux phase with wave vector $(\pi, \pi)$. It has $B_1$ symmetry and a purely imaginary OP in agreement with previous conclusions.

Let us denote the second set of 8 functions by $\tilde{F}_l, l = 1, \ldots, 8$. Each $\tilde{F}_l$ is obtained from $F_l$ by exchanging $e_1$ with $e_3$ and $e_2$ with $e_4$. The linear space spanned by the functions $\tilde{F}_l = 1, \ldots, 8$ yields a reducible representation of $C_{4\pi}$. Decomposing it into its irreducible parts gives one time the representations $A_1, A_2, B_1, B_2$ and two times the representation $E$, exactly as for the first 8 functions $F_l$. The analogue of Eq. (6) reads

$$\tilde{F}(\gamma) = \sum_{l=1}^{8} c_{q_l} \tilde{F}_l,$$  \hspace{1cm} (10)

where the coefficients $c_{q_l}$ are the same as in Table 1. The phase factor $e_j \cdot q_l$ is for all 8 functions equal to $-q$ so that $\gamma$ reads

$$\tilde{F}^*(\gamma) = \pm e^{-i\gamma} \tilde{F}(\gamma).$$  \hspace{1cm} (11)

The same conclusions as above can be drawn from Eq. (11) about the real, imaginary or complex nature of the OPs $\tilde{F}(\gamma)$.

Complex functions for $F(\gamma)$ and $\tilde{F}(\gamma)$ do not necessarily imply that the corresponding states break $T$ symmetry. This is true in particular for our case because a possible imaginary part to $F$ can come from the matrix element but also from combinations of the exponential functions in Eq. (3). A general criterion for an unbroken $T$ symmetry is obtained from the condition that the matrix elements $(c_i^j c_j^i)$ must be real, or equivalently, symmetric if the sites $i$ and $j$ are exchanged. Using Eqs. (2) and (3) one obtains from these two conditions for an unbroken $T$ symmetry,

$$F(q_l, e_j) = e^{-i(q_l \cdot e_j)} F(q_l, -e_j),$$  \hspace{1cm} (12)

and

$$F^*(q_l, e_j) = F(-q_l, e_j).$$  \hspace{1cm} (13)

Inserting Eq. (13) into Eq. (12) yields Eq. (6) which is valid independently whether $T$ symmetry is broken or not. For the special case $q_l = 0$ Eqs. (12) and (13) are compatible with the real OP for the $A_1$ and $B_1$ symmetries, found above, but not with the imaginary OP for the $E$ symmetry. Thus $T$ symmetry is unbroken for the $A_1$ and $B_1$ and broken for the $E$ symmetry. For $q_l = (\pi, \pi)$ one finds that the purely imaginary OPs of the $A_1, B_1$ symmetries break and the real OP of the $E$ symmetry preserves $T$ symmetry. For a general $q_l$ along the diagonals we rewrite the term on the right-hand side of Eq. (13) as $C_2 F(q_l, -e_j)$, multiply this equation with $c_{q_l}$ and sum over $l$ and get

$$\tilde{F}(\gamma) = e^{i\gamma} F(\gamma).$$  \hspace{1cm} (14)

Noting that $F(\gamma)$ and $\tilde{F}(\gamma)$ belong to different subspaces they are linear independent from each other which implies that they are identical zero. This means that the Eqs. (12) and (13), expressing conditions that $T$ is unbroken, are incompatible with the general Eq. (3) for time reversal. Thus we conclude that all the basis functions in Eq. (3) and Eq. (10) break $T$ symmetry for $q \neq 0$ and $\neq (\pi, \pi)$.

The above results differ from those in Refs. [21, 22]. For instance, a charge-ordered, $T$ symmetry conserving state with $q = (q, q)$ is incompatible with our results for any $q$ different from zero and $\pi$. Similarly, we do not see a transition from a $T$ unbroken to a broken state moving along the diagonal from 0 to $(\pi, \pi)$. These discrepancies may be traced back to the different methods used to determine the OP. Ref. [20] chooses and fixes one of the wave vectors of the star in determining the relative motion of electron and hole in the OP. In our view the four fold degeneracy of instability vectors at $T_c$ is lifted below $T_c$ by higher-order interaction terms involving different $q$. This lifting of degeneracy is achieved in our approach by choosing linear combinations of OPs which form basis functions for irreducible representations of $C_{4\pi}$ and $T$. The OP below $T_c$ is thus not related in a simple way to one of the instability vectors of the normal state but contains more than one $q$ even in the plane-wave limit. This can be seen from the following low-order calculation of the OP. The OP dependent part of the mean-field approximation for $H$, Eq. (1), can be written as,

$$H^{MF} = -\frac{V + J}{2} \sum_{q_l, j, k} F^*(q_l, e_j) c_{k+e_j} c_{k+q_l} c_k.$$  \hspace{1cm} (15)
The expectation value \( \langle \epsilon_{k+\mathbf{q}} \rangle \) in Eq. (8) can be expressed in terms of an equal-time Matsubara Green’s function \( G(k, \mathbf{k}+\mathbf{q}) \). Calculating it in third-order in \( H^{MF} \) and using the plane-wave limit one finds

\[
G^{(3)}(k, \mathbf{k}+\mathbf{q}) = \sum_{\mathbf{q'}, \mathbf{e}_j, \mathbf{e}_j'} W(k, \mathbf{q'}, \mathbf{e}_j, \mathbf{e}_j', \mathbf{e}_j''') \cdot F(-\mathbf{q'}, \mathbf{e}_j)F(\mathbf{q'}, \mathbf{e}_j')F(\mathbf{q}, \mathbf{e}_j'''), \tag{16}
\]

where \( W \) is essentially a frequency sum over 4 unperturbed Matsubara Green’s functions. The above expression shows that an OP with momentum \( \mathbf{q} \) couples to all the other wave vectors \( \mathbf{q'} \) of the star and this is even true in the plane-wave limit where only primary instability wave vectors are kept in \( F \).

Next we consider the case of four wave vectors along the crystalline axes, i.e., \( \mathbf{q}_1 = (q,0) \), \( \mathbf{q}_2 = (0,q) \), \( \mathbf{q}_3 = (-q,0) \), and \( \mathbf{q}_4 = (0,-q) \) where \( q \) lies between 0 and \( \pi \). Using the previous notation the functions \( F_l, l = 1, \ldots, 4 \) yield irreducible representations of \( A_1, B_1 \) and \( E \) symmetries with the basis functions \( F_1, F_2, F_3, F_4, F_1 - F_2, F_3 - F_4 \), and \( F_1 - F_3, F_2 - F_4 \), respectively. The exponential factor in Eq. (15) is in each case \( e^{iq} \). Thus Eq. (7) holds for these three representations and their basis functions are complex for \( q \neq 0 \). All the above results also apply to the set \( F_l, l = 1, \ldots, 4 \), if the exponential factor is replaced by \( e^{-iq} \). Thus each of the manifolds \( F \) and \( \tilde{F} \) lead to one \( A_1, B_1 \) and one \( E \) representation and their basis functions are complex for \( q \neq 0 \). The arguments concerning \( T \) breaking around Eqs. (12) and (13) can immediately be transferred to the present star of wave vectors. The result is that all basis functions discussed in this paragraph break \( T \) symmetry for \( q \neq 0 \) or \( \pi \).

The remaining 8 functions are conveniently split into the combinations

\[
F_1^+ = F(q, e_{l+1}) + F(q, e_{l+3}) \quad \text{and} \quad F_1^- = F(q, e_{l+1}) - F(q, e_{l+3})
\]

for \( l = 1, \ldots, 4 \). The functions \( F_1^+, l = 1, \ldots, 4 \) lead to \( A_1, B_1 \) and \( E \), the functions \( F_1^-, l = 1, \ldots, 4 \), to \( A_2, B_2 \) and \( E \) representations. The corresponding basis functions are the same as for the above \( F_1 \) manifold, once \( F_1 \) is replaced by \( F_1^+ \) or \( F_1^- \), respectively. For all 8 functions the wave and the bond vectors are perpendicular to each other implying that \( q \) is identical to zero and that no complex exponential appears in Eq. (12). As a result we get \( F^+ (\gamma) = C_2 F^+ (\gamma) \) so that \( F^+ (\gamma) \) is real for \( \gamma = A_1, B_1 \) and imaginary for \( \gamma = E \). It is easy to see that these results are compatible with Eq. (12), i.e., with the assumption of an unbroken \( T \) symmetry. Alternatively, one can use Eq. (13) to obtain \( F^+ (\gamma) = C_2 F^+(\gamma) \), i.e., the same relation as from Eq. (5), which means that the above basis functions indeed exhibit \( T \) symmetry. Finally, let us consider the basis functions \( F^-(\gamma) \) of the irreducible representations \( \gamma = A_2, B_2, E \). The general Eq. (5) yields \( F^-(\gamma) = C_2 F^-(\gamma) \) implying that \( F^- (A_2) \) and \( F^- (B_2) \) are real and \( F^- (E) \) are imaginary. If \( T \) symmetry is unbroken Eq. (12) must be valid. However, this equation yields \( F^- (\gamma) = 0 \) for \( \gamma = A_2, B_2, E \) in contradiction with the above general non-vanishing expressions. Thus the assumption of an unbroken \( T \) symmetry for these three states must be wrong and \( T \) symmetry is broken.

For completeness let us consider the case of an usual CDW without internal bond degrees of freedom. Eq. (5) reads for \( e_j = 0 \) \( F^+(q) = C_2 F(q) \) which is identical with \( F^+(q) = F(-q) \) from Eq. (13). It follows that \( T \) symmetry is always unbroken in an usual CDW.

The above analysis showed that many of the symmetry allowed charge OPs break \( T \) symmetry. The finite imaginary part of these OPs generate circulating currents and space-dependent magnetic fields [15, 26] which so far could not be observed [27, 29]. Concentrating therefore on \( T \) conserving OPs there are none of this kind in the case of a star with wave vectors along the diagonals. For the experimentally observed star with wave vectors along the crystalline axes there are three OPs which preserve \( T \) symmetry. They have the symmetries \( A_1, B_1 \), and \( E \) and originate from the \( F^+ \) manifold. The explicit basis functions of the first two symmetries are \( 4 \sum_k (\cos k_x \Re ((\epsilon_{k+q_1}^\dagger \epsilon_{k+q_2})) \pm \cos k_y \Re ((\epsilon_{k+q_3}^\dagger \epsilon_{k+q_4})) \), where the upper and lower signs refer to the momenta characterizing the intra- and inter-cell behavior of the OP, i.e., \( q_x \) appears together with \( k_y \) and \( q_y \) with \( k_x \). The basis functions for the \( E \) symmetry are \( 4i \sum_k \cos k_x \Im ((\epsilon_{k+q_1}^\dagger \epsilon_{k+q_2})) \) and \( 4i \sum_k \cos k_y \Im ((\epsilon_{k+q_3}^\dagger \epsilon_{k+q_4})) \). They describe uni-directional charge order, again with strong correlations between intra- and inter-cell degrees of freedom. If the experimental OP preserves \( T \) symmetry it must be identical with one of these last three OPs.

The OP deduced from experimental data in Ref. [8] exhibits \( B_1 \) and \( A_1 \) symmetry in the \( e_j \) and \( \mathbf{q}_1 \) variables, respectively. In our notation it thus should be identified with

\[
\tilde{F} = \sum_{k, l, j} (\epsilon_{k+q_1}^\dagger \epsilon_{k+q_2}) e^{i k e_j} (-1)^{l+1}, \tag{17}
\]

which is equal to \( F(B_1) + \tilde{F}(B_1) - F^+(B_1) \). The last function is real and preserves \( T \) whereas the first two are complex and break \( T \) symmetry. The total function \( \tilde{F} \) is thus also complex and breaks \( T \) symmetry. On the other hand, Ref. [8] adopts the approximation

\[
F(q, e_j) \rightarrow e^{-i q / 2} \sum_k \Delta(k)e^{i e_j} k, \tag{18}
\]

i.e., after shifting the sum over \( k \) by \(-q / 2\) the matrix element in \( F \) is approximated by the real and \( \mathbf{q} \) independent function \( \Delta(k) \). If \( \Delta(k) \) is an even function of \( k \) the modified functions \( F \) of Eq. (18) satisfy Eq.
and thus preserve $T$ symmetry. Inserting Eq. (18) into $F(B_1) + \tilde{F}(B_1) - F^+(B_1)$ yields $\hat{F} = 4(\cos q/2 + 1) \sum_k \Delta(k)(\cos k_x - \cos k_y)$, in agreement with Ref. [8]. Note that $\hat{F}$ becomes real and $T$ symmetric only after the approximation leading to Eq. (18). This approximation, however, is not acceptable because it also yields the relation $Re F(B_1) = Re \tilde{F}(B_1)$ or $TF(B_1) = \tilde{F}(B_1)$ which contradicts the assumed linear independence of the basis functions in Eq. (3). Independently of the approximation Eq. (18), $\hat{F}$ is only real if the above condition $T F(B_1) = \tilde{F}(B_1)$ is satisfied. Thus a real and $T$ symmetric OP of the form of Eq. (17), as has been assumed in Ref. [3], is not compatible with the underlying symmetries.

In conclusion, we have identified all symmetry allowed bond OPs for any model with nearest neighbor interactions such as the $t$-$J$ model and studied their properties, in particular, with respect to time reversal. The obtained results are relevant for recently observed charge-ordered states in underdoped cuprates and their symmetries. They also hold in the presence of strong electronic correlations. The proposed OPs are at variance with variational Ansätze used in the past both in theoretical and experimental studies. Being based on rigorous group theoretical considerations our results are useful to design improved variational forms for the OP in microscopic calculations or to the interpretation of experimental data.

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