Comment on

“Symmetry classification of bond order parameters in cuprates”

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We review the transformation of bond order waves with non-trivial form factors
under time-reversal and point group symmetry. Zeyher (arXiv:1406.6846) argues
that certain $d$-form factor states must be “flux states”, but this does not apply to
the form factors as defined by us (arXiv:1402.4807). The latter definitions were used
in the experimental detection (arXiv:1402.5415, arXiv:1404.0362).
I. INTRODUCTION

A recent STM experiment \cite{1} has presented sublattice-resolved information on the density wave order in the underdoped cuprates, including a direct phase-sensitive identification of a $d$-form factor. X-ray experiments have also reported evidence for such a form-factor \cite{2}.

In this note we reiterate and clarify symmetry aspects of such form factors, and specifically their transformation properties under time-reversal and point group symmetry. It is useful to define the generalized bilinear order parameter $\Delta_{ij}$ by \cite{3–11}

$$\Delta_{ij} \equiv < c_{i\alpha}^\dagger c_{j\alpha} >$$

$$= \sum_Q \left[ \frac{1}{V} \sum_k e^{i k \cdot (r_i - r_j)} \Delta_Q(k) \right] e^{i Q \cdot (r_i + r_j)/2},$$

with $i, j$ labels for the Cu sites of the square lattice at spatial co-ordinates $r_i, r_j$, and $c_{i\alpha}$ is the electron annihilation operator with spin label $\alpha = \uparrow, \downarrow$. The wavevectors of the density wave orders are $Q$, and $\Delta_Q(k)$ are the corresponding form factors which are complex functions of the wavevector $k$ extending over the first Brillouin zone. The volume of the system is $V$.

In momentum space, we can write Eq. (1) as

$$\Delta_Q(k) = < c_{k-Q/2,\alpha}^\dagger c_{k+Q/2,\alpha} >.$$  (2)

Taking the Hermitian conjugate of Eq. (1), we note that every such order parameter must satisfy

$$\Delta_{ij} = \Delta_{ji}^*$$  (3)

which immediately implies that

$$\Delta_Q^*(k) = \Delta_{-Q}(k).$$  (4)

Then, we note that under time-reversal, $T$, we have

$$T: \ \Delta_{ij} \rightarrow \Delta_{ij}^*.$$  (5)

The combination of Eqs. (1,3,4,5) is now seen to imply

$$T: \ \Delta_Q(k) \rightarrow \Delta_Q(-k) = \Delta_{-Q}^*(-k).$$  (6)

It is this simple time-reversal transformation which is the main advantage of the parameterization in Eq. (1).
In contrast, numerous other works \cite{12-17}, including the recent work of Zeyher \cite{18}, use a parametrization of the form
\[
\Delta_{ij} = \sum_Q \left[ \frac{1}{V} \sum_k F_Q(k) e^{iQ(r_i - r_j)} \right] e^{iQ \cdot r_i},
\] (7)
or equivalently
\[
F_Q(k) = \langle c_{k,\alpha}^\dagger c_{k+Q,\alpha} \rangle.
\] (8)
Comparing Eqs. (1) and (7) we can conclude that
\[
F_Q(k - Q/2) = \Delta_Q(k).
\] (9)
Thus the “d-wave flux” state \cite{13, 14}, which has \(Q = (\pi, \pi)\) and \(F_Q(k) \sim \cos(k_x) - \cos(k_y)\), is a p-form factor state in our notation, with \(\Delta_Q(k) \sim \sin(k_x) - \sin(k_y)\). Also, note that now
\[
F_Q^*(k) = F_{-Q}(k + Q),
\] (10)
and under time-reversal
\[
\mathcal{T} : F_Q(k) \rightarrow F_Q(-k - Q) = F_{-Q}^*(-k).
\] (11)
From Eq. (11) we see that a d-form factor \cite{15, 17}
\[
F_Q(k) \sim \cos(k_x) - \cos(k_y)
\] (12)
is not invariant under time-reversal for general \(Q\), as has been noted by Zeyher \cite{18}. However, precisely for this reason, we have consistently used \cite{1, 3-7} Eq. (1) rather than Eq. (7): the d-form factor
\[
\Delta_Q(k) \sim \cos(k_x) - \cos(k_y)
\] (13)
is indeed invariant under time-reversal for all \(Q\), as is evident from Eq. (6). Note that the \(\mathcal{T}\)-preserving form factor in Eq. (13), when expressed in terms of \(F_Q(k)\) using Eq. (9), yields a function \(F_Q(k)\) which does not transform under an irreducible representation of the point group, but is a mixture of d- and p-form factors.

\section{II. POINT GROUP SYMMETRY}
Zeyher \cite{18} classifies the functions \(F_Q(k)\) in terms of irreducible point-group representations, but this does not commute with time-reversal. Here, we consider a point-group classification of \(\Delta_Q(k)\) and show by explicit construction that
• time reversal invariant, $d$-form factor bond order waves form bases for irreducible representations of the point group of the square lattice,

• some of these representations contain unidirectional (single wavevector) waves.

This is important because of the following argument. In a second order phase transition that breaks a symmetry group $G$, close to the critical point in the symmetry broken phase, the order parameter $\Phi$ is very small, and hence transforms under a linear representation $\Gamma$ of $G$:

$$ g \in G : \quad \Phi_i \mapsto \Gamma(g)_{ij} \Phi_j. \quad (14) $$

If we further assume that $\Gamma$ is unitary, then it must also be irreducible. In fact, we can always decompose the representation $\Gamma$ in irreducible representations, and, expanding the free energy to quadratic order, we have

$$ F = F_0 + \sum_{r,s} [\Phi_i^{(r)}]^* c_{ij}^{rs} \Phi_j^{(s)}, \quad (15) $$

where $\Phi^{(r)}$ transforms under an irreducible representation $\Gamma_r$ of $G$. Since the free energy must be invariant under $G$, by Shur’s lemma we have

$$ c_{ij}^{rs} = c_r \delta_{ij} \delta_{rs}, \quad F = F_0 + \sum_r c_r [\Phi_i^{(r)}]^* \Phi_i^{(r)}. \quad (16) $$

For a generic, non fine-tuned phase transition, only one of the $c_r$ changes sign, and hence the order parameter transforms under the irreducible representation $\Gamma_r$.

To be self contained, let us briefly summarize properties of the symmetry group of the square $C_4$. The group is generated by $R$, a rotation of $\pi/2$ and $P$, the reflection about the $y$ axis. It contains 8 elements

$$ C_4 = \{1, R, R^2, R^3, P, RP, R^2P, R^3P\}. \quad (17) $$

It has 4 inequivalent irreducible representations:

1. The faithful, 2 dimensional representations $\Gamma_f$,

$$ \Gamma_f(R) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \Gamma_f(P) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (18) $$

which is just a subgroup of $O(2)$.
2. A one-dimensional representation $\Gamma_p$ in which the normal subgroup $\{1, R, R^2, R^3\}$ is mapped to the identity

$$\Gamma_p(R) = 1, \quad \Gamma_p(P) = -1. \quad (19)$$

3. A one-dimensional representation $\Gamma_r$ in which the normal subgroup $\{1, R^2, P, R^2 P\}$ is mapped to the identity

$$\Gamma_r(R) = -1, \quad \Gamma_r(P) = 1. \quad (20)$$

4. The trivial, one-dimensional representation $\Gamma_0(P) = \Gamma_0(R) = 1.$

FIG. 1. Basis functions with wavevector parallel to the axis, for $Q = \pi/5.$
It is convenient to think about the problem in real space. Let us consider the following basis functions for the order parameter $\Delta_{r,r'} = \langle c^+_r c_{r'} \rangle$:

\[
\Delta^1_{r,r+\hat{a}} = \cos Q \left( r \cdot \hat{x} + \frac{1}{2} \right), \quad \Delta^1_{r,r+\hat{g}} = -\cos Q r \cdot \hat{x}, \quad (21)
\]
\[
\Delta^2_{r,r+\hat{a}} = \sin Q \left( r \cdot \hat{x} + \frac{1}{2} \right), \quad \Delta^2_{r,r+\hat{g}} = -\sin Q r \cdot \hat{x}, \quad (22)
\]
\[
\Delta^3_{r,r+\hat{a}} = \cos Q r \cdot \hat{y}, \quad \Delta^3_{r,r+\hat{g}} = -\cos Q \left( r \cdot \hat{y} + \frac{1}{2} \right), \quad (23)
\]
\[
\Delta^4_{r,r+\hat{a}} = \sin Q r \cdot \hat{y}, \quad \Delta^4_{r,r+\hat{g}} = -\sin Q \left( r \cdot \hat{y} + \frac{1}{2} \right). \quad (24)
\]

These basis functions are illustrated in fig. [1]. They are all real and hence they do not break time reversal. They are unidirectional, $d$-form factor bond order waves. $\Delta^1$ and $\Delta^2$ have wavevector parallel to the $x$ axis and differ by a phase. In the same way, $\Delta^3$ and $\Delta^4$ have wavevector parallel to the $y$ axis and differ by a phase. These four functions support a reducible representation of the point group:

\[
P\Delta^1 = \Delta^1, \quad P\Delta^2 = -\Delta^2, \quad P\Delta^3 = \Delta^3, \quad P\Delta^4 = \Delta^4, \quad (25)
\]
\[
R\Delta^1 = -\Delta^3, \quad R\Delta^2 = -\Delta^4, \quad R\Delta^3 = -\Delta^1, \quad R\Delta^4 = \Delta^2. \quad (26)
\]

This representation is decomposed in irreducible representations as follows:

- $\{\Delta^2, \Delta^4\}$ is a basis for the faithful representation $\Gamma_f$.
- $\{\Delta^1 + \Delta^3\}$ is a basis for $\Gamma_t$.
- $\{\Delta^1 - \Delta^3\}$ is a basis for the trivial representation $\Gamma_0$.

The two basis $\{\Delta^1 + \Delta^3\}, \{\Delta^1 - \Delta^3\}$ are shown in fig. [2].

The same procedure can be carried out for bond order waves with diagonal wavevector. Let us consider the following basis functions:

\[
\Delta^5_{r,r+\hat{a}} = \cos Q \left( r \cdot \hat{x} + r \cdot \hat{y} + \frac{1}{2} \right), \quad \Delta^5_{r,r+\hat{g}} = -\cos Q \left( r \cdot \hat{x} + r \cdot \hat{y} + \frac{1}{2} \right), \quad (27)
\]
\[
\Delta^6_{r,r+\hat{a}} = \sin Q \left( r \cdot \hat{x} + r \cdot \hat{y} + \frac{1}{2} \right), \quad \Delta^6_{r,r+\hat{g}} = -\sin Q \left( r \cdot \hat{x} + r \cdot \hat{y} + \frac{1}{2} \right), \quad (28)
\]
\[
\Delta^7_{r,r+\hat{a}} = \cos Q \left( r \cdot \hat{x} - r \cdot \hat{y} + \frac{1}{2} \right), \quad \Delta^7_{r,r+\hat{g}} = -\cos Q \left( r \cdot \hat{x} - r \cdot \hat{y} - \frac{1}{2} \right), \quad (29)
\]
\[
\Delta^8_{r,r+\hat{a}} = \sin Q \left( r \cdot \hat{x} - r \cdot \hat{y} + \frac{1}{2} \right), \quad \Delta^8_{r,r+\hat{g}} = -\sin Q \left( r \cdot \hat{x} - r \cdot \hat{y} - \frac{1}{2} \right). \quad (30)
\]
These basis functions are illustrated in fig. 3. They are all real and hence they do not break time reversal. They are unidirectional, $d$-form factor bond order waves. $\Delta^5$ and $\Delta^6$ have wavevector parallel to $\hat{x} + \hat{y}$ and differ by a phase. In the same way, $\Delta^7$ and $\Delta^8$ have wavevector parallel to $\hat{x} - \hat{y}$ and differ by a phase. These four functions support a reducible representation of the point group:

\[
P \Delta^5 = \Delta^7, \quad P \Delta^6 = -\Delta^8, \quad (31)
\]

\[
R \Delta^5 = -\Delta^7, \quad R \Delta^6 = \Delta^8, \quad R \Delta^7 = -\Delta^5, \quad R \Delta^8 = -\Delta^6. \quad (32)
\]

This representation is decomposed in irreducible representations as follows:

- $\{\Delta^6, \Delta^8\}$ is a basis for the faithful representation $\Gamma_f$. More precisely, the representation matrices have the form (18) in the basis $\{\Delta^6 + \Delta^8, \Delta^6 - \Delta^8\}$.

- $\{\Delta^5 + \Delta^7\}$ is a basis for $\Gamma_r$.

- $\{\Delta^5 - \Delta^7\}$ is a basis for the trivial representation $\Gamma_0$.

The two basis $\{\Delta^5 + \Delta^7\}, \{\Delta^5 - \Delta^7\}$ are shown in fig. 4. With reference to these two order parameters, the irreducible representation argument would tell us that the either the order $\Delta^5 + \Delta^7$ or $\Delta^5 - \Delta^7$ develops. However, by looking at fig. 4, it is clear that they
FIG. 3. Basis functions with diagonal wavevector, for $Q = \pi/5$.

are almost the same upon translation. They would be exactly the same if the wavevector had been chosen incommensurate. This means that the free energy splitting between the two irreducible representations is just a commensuration effect, and hence goes to zero as the commensuration period grows. This makes it clear that the irreducible representation argument is not of the greatest physical relevance in this context.

Zeyher discusses how from possible degenerate ordering vectors $Q$ a particular order develops. This depends on the parameters of an expansion of the Landau free energy. The Landau free energy only has $N$’th order terms of the form

$$
\prod_{i=1}^{N} \Delta_{Q_i}(k_i)
$$

(33)
where translational symmetry requires that

\[ \sum_{i=1}^{N} Q_i = 0 \]  

(34)

for every term (up to reciprocal lattice vectors). So a state with incommensurate wavevectors \( Q = (q, q) \) and \( -Q \) will not necessarily generate density waves at \( Q' = (q, -q) \) because there are no terms which are linear in \( \Delta_Q(k') \) in Eq. (33).

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