

Thesis Title

Dissertation of

Your Name

27th of September, 2024

Advisor: Prof. Dr. Your Advisor

Thesis Title

Zur Erlangung des akademischen Grades eines
DOKTORS/DOKTORIN DER NATURWISSENSCHAFTEN
(Dr. rer. nat.)

von der KIT-Fakultät für Physik des
Karlsruher Instituts für Technologie (KIT)
eingereichte/angenommene

Dissertation

von
M.Sc. Your Name
aus Birthplace

Tag der mündlichen Prüfung: 15. 11. 2024.
Referent: Prof. Dr. First Referee
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Dedication

Summary and Overview

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1

Chapter 1

First chapter

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1.1 First section

Magnetism most commonly arises from interactions related to the spin degrees of freedom [1, 2]. The corresponding order parameter S has a non-trivial structure in spin space and is odd under time reversal (TR):

$$\hat{\Theta}^{-1} S \hat{\Theta} = -S, \quad (1.1)$$

where $\hat{\Theta}$ is the antiunitary many-body TR operator. The simplest S is, of course, spin itself, which is the appropriate order parameter for a ferromagnet. However, there is a wide variety of orbital and spin structures that the order parameter S may acquire, depending on the type of spin magnetism. A comprehensive classification of possible spin-magnetic orders is provided in Fig. 1.1, reproduced from Ref. [3]. This classification is based on the local orientation of the spin moments and the symmetry of the overall spin pattern.

In correlated systems, magnetism may develop in the orbital sector as well [4, 5]. Such orbital magnetism is characterized by “generalized orbital angular momentum” or “flux” operators L which are odd under time reversal,

$$\hat{\Theta}^{-1} L \hat{\Theta} = -L, \quad (1.2)$$

but have trivial spin structures. As we shall later in Sec. 1.1.1 see, this difference in the spin structure has far-reaching consequences, especially when SOC is weak, and it is the main reason for why ferromagnetic and IUC LC fluctuations behave so differently near their QCPs. The range of possible LC orders is, in principle, as varied as that of spin-magnetic orders classified in Fig. 1.1. However, LC order is less common than spin magnetism, which is why its phases have not been explored as extensively.

1.1.1 First subsection

The only way TR symmetry can be broken in the charge or orbital sector is through the formation of some sort of charge currents. This pattern of spontaneously flowing currents, moreover, must be made of closed loops to avoid a global current, which is forbidden because of a theorem first proved by Bloch [6–11]. Here we in addition prove a generalized Bloch-Kirchhoff theorem according to which the pattern of spontaneously flowing currents must be divergenceless, i.e., respect Kirchhoff’s law and not lead to an accumulation of charge in some

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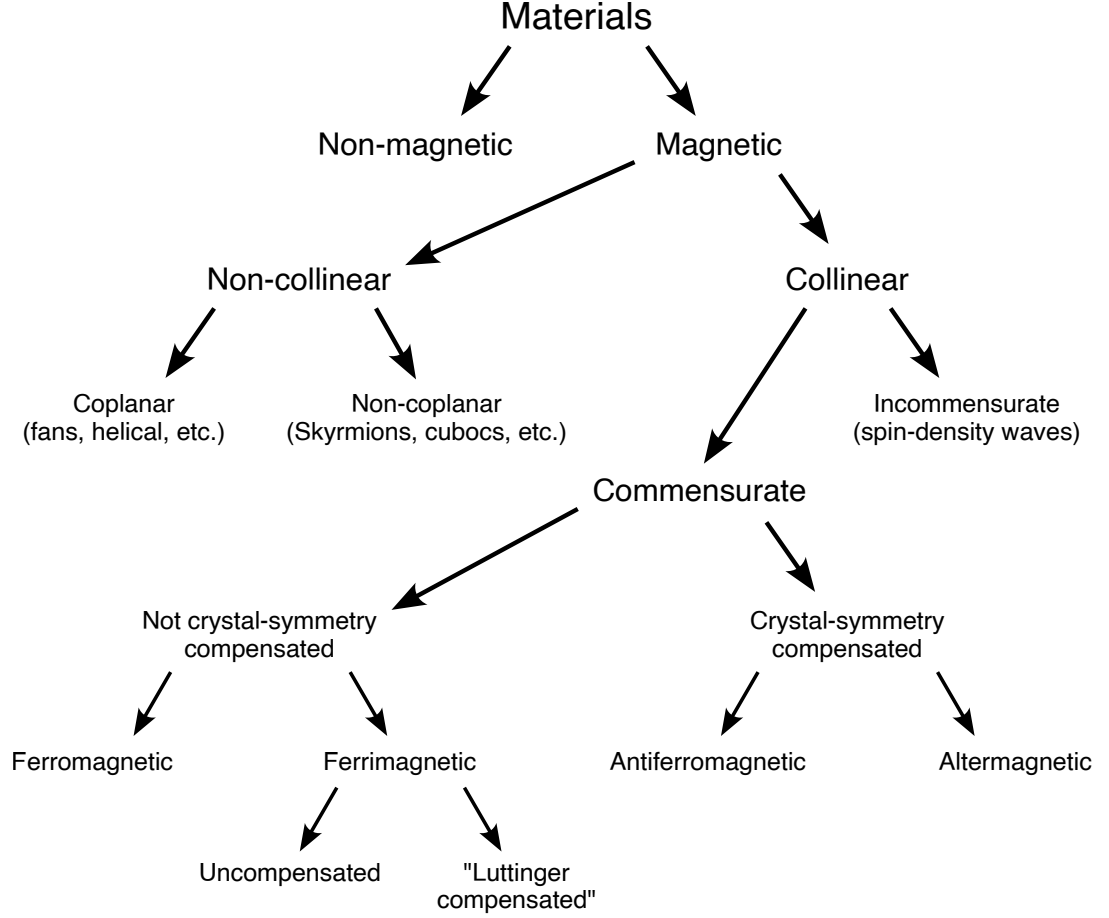


Figure 1.1: **Classification of spin-magnetic orders according to symmetry and orientation of the local spin moments** [3]. Magnetism is characterized by the breaking of time-reversal (TR) symmetry Θ . The local spins can either be collinear (aligned along one axis), coplanar (orthogonal to one axis), or non-coplanar. Furthermore, the pattern of the local spins and magnetic moments can either be commensurate (have the same periodicity as the underlying lattice) or incommensurate (break additional translation symmetries). Even though TR symmetry is broken, composing TR with a crystal symmetry may leave the spin pattern invariant and thus compensate for TR symmetry-breaking. Antiferromagnets are compensated by translations, whereas altermagnets are compensated by point group operations such as reflections or rotations. Spatial-inversion symmetry is always preserved by spin-magnetic order.

parts of the system. The latter was previously invoked in Ref. [12] in the form of Kirchhoff constraints, but not rigorously proved in the same manner as Bloch's theorem. These two theorems give fundamental constraints on the possible thermodynamically stable LC orders which may arise in nature.

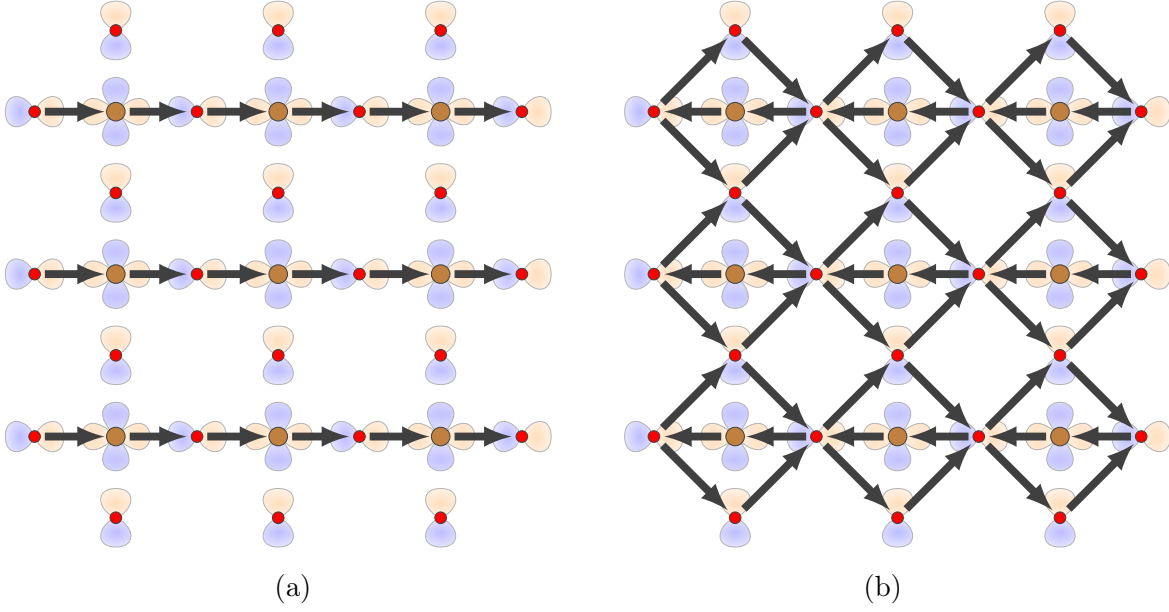


Figure 1.2: **Examples of loop-current (LC) patterns that have a finite (a) and vanishing (b) global charge current.** Arrows indicate the direction of the local currents, i.e., the flow of charge between the orbitals. The underlying model is the three-orbital tight-binding model of the copper planes of the cuprates which we study in the next chapter. The LC pattern shown under (a) is forbidden by Bloch's theorem [6–11], as discussed in the text. As for the currents under (b), they must not lead to any local accumulation of charge, as proved in the text.

1.1.1.1 First subsection

The proof of Bloch's theorem proceeds by contradiction. Let us assume that a ground state $|\Psi_0\rangle$ of energy $E_0 = \langle \Psi_0 | \mathcal{H} | \Psi_0 \rangle$ has a finite global electron charge current $\mathbf{J} = \int_{\mathbf{r}} \langle \Psi_0 | \mathbf{j}_e | \Psi_0 \rangle$, where $\int_{\mathbf{r}} = \int d^d r$. The corresponding charge is locally conserved in the sense that $\partial_t \rho_e + \nabla \cdot \mathbf{j}_e = 0$, where ρ_e is the local charge density operator of the electrons only and $\partial_t \rho_e = i[\mathcal{H}, \rho_e]/\hbar$. We use Heisenberg's picture throughout. Now consider the state

$$|\Psi'_0\rangle = \exp\left(i \int_{\mathbf{r}} \mathbf{k} \cdot \mathbf{r} \rho_e\right) |\Psi_0\rangle \quad (1.3)$$

for small \mathbf{k} . This corresponds to a state in which every electron has been given an additional momentum $\hbar\mathbf{k}$. To linear order in \mathbf{k} , its energy equals

$$\begin{aligned}
E'_0 &= \langle \Psi'_0 | \mathcal{H} | \Psi'_0 \rangle \\
&= E_0 + i \int_{\mathbf{r}} \mathbf{k} \cdot \mathbf{r} \langle \Psi_0 | [\mathcal{H}, \rho_e] | \Psi_0 \rangle + \mathcal{O}(\mathbf{k}^2) \\
&= E_0 + \hbar \int_{\mathbf{r}} \mathbf{k} \cdot \mathbf{r} \langle \Psi_0 | \partial_t \rho_e | \Psi_0 \rangle + \mathcal{O}(\mathbf{k}^2) \\
&= E_0 - \hbar \int_{\mathbf{r}} \mathbf{k} \cdot \mathbf{r} \nabla \cdot \langle \Psi_0 | \mathbf{j}_e | \Psi_0 \rangle + \mathcal{O}(\mathbf{k}^2) \\
&= E_0 + \hbar \mathbf{k} \cdot \int_{\mathbf{r}} \langle \Psi_0 | \mathbf{j}_e | \Psi_0 \rangle + \mathcal{O}(\mathbf{k}^2) \\
&= E_0 + \hbar \mathbf{k} \cdot \mathbf{J} + \mathcal{O}(\mathbf{k}^2).
\end{aligned} \tag{1.4}$$

Hence we may always lower the energy relative to E_0 by orienting \mathbf{k} in the opposite direction of \mathbf{J} . This implies that the true ground state cannot have a finite global electron charge current [6]. Notice how the coupling to the ions, which proceeds via the density ρ_e , drops out in the above manipulations. Examples of LC patterns which do and do not respect Bloch's theorem are provided in Fig. 1.2.

This proof applies to continuum models at zero temperature subject to open boundary conditions. All three of these assumptions can be lifted [7–11]. In the case of lattice models, the local charge conservation law takes the form

$$\partial_t \rho_{\mathbf{R}\alpha} + \sum_{\mathbf{R}'\alpha'} j_{\mathbf{R}\alpha; \mathbf{R}'\alpha'} = 0, \tag{1.5}$$

where $j_{\mathbf{R}\alpha; \mathbf{R}'\alpha'} = j_{\mathbf{R}\alpha; \mathbf{R}'\alpha'}^\dagger = -j_{\mathbf{R}'\alpha'; \mathbf{R}\alpha}$ is the current flowing from the lattice site \mathbf{R} and orbital α to the lattice site \mathbf{R}' and orbital α' . The variation

$$|\Psi'_0\rangle = \exp\left(i \sum_{\mathbf{R}\alpha} \mathbf{k} \cdot \mathbf{R} \rho_{\mathbf{R}\alpha}\right) |\Psi_0\rangle \tag{1.6}$$

results in an identical $E'_0 = E_0 + \hbar \mathbf{k} \cdot \mathbf{J} + \mathcal{O}(\mathbf{k}^2)$, where the global current is defined as

$$\mathbf{J} = \frac{1}{2} \sum_{\mathbf{R}\alpha \mathbf{R}'\alpha'} (\mathbf{R}' - \mathbf{R}) \langle \Psi_0 | j_{\mathbf{R}\alpha; \mathbf{R}'\alpha'} | \Psi_0 \rangle. \tag{1.7}$$

In the proof for a finite-temperature ensemble described by the density matrix $\rho_0 = \mathcal{Z}^{-1} e^{-\beta \mathcal{H}}$, where $\mathcal{Z} = \text{Tr } e^{-\beta \mathcal{H}}$, one considers the variation

$$\rho_0 \rightarrow \rho'_0 = \exp\left(i \int_{\mathbf{r}} \mathbf{k} \cdot \mathbf{r} \rho_e\right) \rho_0 \exp\left(-i \int_{\mathbf{r}} \mathbf{k} \cdot \mathbf{r} \rho_e\right) \tag{1.8}$$

and by completely analogous manipulations obtains that the free energy $F' = F + \hbar \mathbf{k} \cdot \mathbf{J} + \mathcal{O}(\mathbf{k}^2)$ given by $F = \text{Tr } \rho_0 (\mathcal{H} + k_B T \log \rho_0)$ is not minimal. Finally, for periodic boundary conditions the variational \mathbf{k} is on the order of L^{-1} , where L is the length of the system. Because \mathbf{k} is not infinitesimal, the quadratic term in the expansion of E_0 is non-negligible and, because

Table 1.1: **A selected list of bulk orders, classified according to whether they break translation (red) or time-reversal (TR) symmetry and whether they are trivial or not in the spin sector.** Orbital/charge orders are trivial in spin space. Highlighted in red are orders which break translation invariance. Nematic orders are electronic orders which spontaneously break point group symmetries such as rotations or reflections without breaking parity or translation symmetry [13, 14]. Spin-nematics do the same in the spin sector, but without TR symmetry-breaking [15, 16]. Ferroelectrics have spontaneous electric polarizations and their modes are usually soft polar phonons [17]. Alterelectrics I dub orders which break parity in the orbital sector, just like ferroelectrics, but whose order parameter does not transform like a vector. Hence, alterelectrics do not have a net electric dipole moment. Charge- and spin-density waves are spontaneously forming periodic modulations of the charge or spin density which are incommensurate with the underlying lattice [18, 19]. Loop-current order is orbital magnetism. Spin loop currents are loop currents which carry spin. Regarding the spin-magnetic orders, see Fig. 1.1 for an explanation. For a more systematic classification of orders, see Refs. [20–22].

	orbital or charge	spin
TR-even	nematic ferroelectric alterelectric charge-density waves	spin-nematic intra-unit-cell spin loop currents staggered spin loop currents
TR-odd	intra-unit-cell (orbital) loop currents staggered (orbital) loop currents	ferromagnetic altermagnetic antiferromagnetic spin-density waves

it is positive, it can compensate for the linear term and allow for a global charge current density which is on the order of L^{-1} . The global charge current density thus vanishes in the thermodynamic limit.

Because the proof only relies on the local conservation of charge, Bloch's theorem quite generally applies to $U(1)$ symmetries and their Noether currents [11]. In particular, in the absence of spin-orbit coupling global spin currents are forbidden in the ground state as well.

A

Appendix A

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A.1 First subsection

Suppose we are given two vectors $\mathbf{v} = (v_1, \dots, v_N)^\top$ and $\mathbf{u} = (u_1, \dots, u_M)^\top$ which transform under the representations \mathcal{M}_v and \mathcal{M}_u of a finite group G , respectively. Then the composite object $\{v_a u_b\}$ transforms like

$$g: v_a u_b \mapsto \sum_{c=1}^N \sum_{d=1}^M [\mathcal{M}_v(g)]_{ac} [\mathcal{M}_u(g)]_{bd} v_c u_d, \quad (\text{A.1})$$

which is fairly complicated. We want to simplify this.

The first step is to introduce the direct-product vector

$$\mathbf{v} \otimes \mathbf{u} = \begin{pmatrix} v_1 u_1 \\ \vdots \\ v_1 u_M \\ v_2 u_1 \\ \vdots \\ v_N u_M \end{pmatrix}. \quad (\text{A.2})$$

Then Eq. (A.1) can be recast into matrix multiplication with the direct-product matrix $\mathcal{M}_v(g) \otimes \mathcal{M}_u(g)$:

$$g: \mathbf{v} \otimes \mathbf{u} \mapsto [\mathcal{M}_v(g) \otimes \mathcal{M}_u(g)](\mathbf{v} \otimes \mathbf{u}) = [\mathcal{M}_v(g)\mathbf{v}] \otimes [\mathcal{M}_u(g)\mathbf{u}]. \quad (\text{A.3})$$

Table A.1: **The character table of the tetragonal point group D_{4h}** [23]. The irreps are divided according to parity into even (subscript g) and odd (u) ones. C_4 are 90° rotations around \hat{e}_z . C_2 , C'_2 , and C''_2 are 180° rotations around \hat{e}_z , \hat{e}_x or \hat{e}_y , and the diagonals $\hat{e}_x \pm \hat{e}_y$, respectively. P is space inversion or parity. Improper rotations S_4 and mirror reflections Σ_h , Σ'_v , and Σ''_d are obtained by composing C_4 , C_2 , C'_2 , and C''_2 with P , respectively.

D_{4h}	E	$2C_4$	C_2	$2C'_2$	$2C''_2$	P	$2S_4$	Σ_h	$2\Sigma'_v$	$2\Sigma''_d$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1
E_g	2	0	-2	0	0	2	0	-2	0	0
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1
E_u	2	0	-2	0	0	-2	0	2	0	0

Hence $\mathbf{v} \otimes \mathbf{u}$ transforms under $\mathcal{M}_v \otimes \mathcal{M}_u$.

The components of \mathbf{v} and \mathbf{u} can be scalars or operators. In the case of operators, there is usually a representation of G on the operator space, call it $\hat{\mathcal{U}}$, which is related to the representations \mathcal{M}_v and \mathcal{M}_u through:

$$\hat{\mathcal{U}}^{-1}(g)v_a\hat{\mathcal{U}}(g) = \sum_{b=1}^N [\mathcal{M}_v(g)]_{ab}v_b, \quad (\text{A.4})$$

$$\hat{\mathcal{U}}^{-1}(g)u_a\hat{\mathcal{U}}(g) = \sum_{b=1}^M [\mathcal{M}_u(g)]_{ab}u_b. \quad (\text{A.5})$$

Notice how these relations are consistent with composition ($g \rightarrow g_1g_2$) and how

$$\hat{\mathcal{U}}^{-1}(g)v_a u_b \hat{\mathcal{U}}(g) = \hat{\mathcal{U}}^{-1}(g)v_a \hat{\mathcal{U}}(g) \hat{\mathcal{U}}^{-1}(g)u_b \hat{\mathcal{U}}(g) = \sum_{c=1}^N \sum_{d=1}^M [\mathcal{M}_v(g)]_{ac} [\mathcal{M}_u(g)]_{bd} v_c u_d. \quad (\text{A.6})$$

The next step in the simplification is to decompose $\mathcal{M}_v \otimes \mathcal{M}_u$ into irreps. More explicitly, we want to change into a basis in which $\mathcal{M}_v \otimes \mathcal{M}_u$ is block diagonal:

$$\begin{aligned} \mathcal{B}^{-1} \mathcal{M}_v(g) \otimes \mathcal{M}_u(g) \mathcal{B} &= \begin{pmatrix} \mathcal{M}_{\zeta_1}(g) & & & \\ & \mathcal{M}_{\zeta_2}(g) & & \\ & & \mathcal{M}_{\zeta_3}(g) & \\ & & & \ddots \end{pmatrix} \\ &= (\mathcal{M}_{\zeta_1} \oplus \mathcal{M}_{\zeta_2} \oplus \mathcal{M}_{\zeta_3} \oplus \dots)(g). \end{aligned} \quad (\text{A.7})$$

Although finding \mathcal{B} is a bit involved, finding out which ζ_1, ζ_2, \dots irreps appear on the right-hand side is more straightforward since it can be deduced from the characters alone. By taking the trace of the above, one finds that

$$\chi_{\mathcal{M}_v \otimes \mathcal{M}_u}(g) = \chi_{\mathcal{M}_v}(g)\chi_{\mathcal{M}_u}(g) = \chi_{\mathcal{M}_{\zeta_1}}(g) + \chi_{\mathcal{M}_{\zeta_2}}(g) + \chi_{\mathcal{M}_{\zeta_3}}(g) + \dots \quad (\text{A.8})$$

Given that we know the characters of \mathcal{M}_v , \mathcal{M}_u , and all the irreps, the above is readily solved to find which irreps appear in the decomposition of $\mathcal{M}_v \otimes \mathcal{M}_u$. The orthogonality of irreps is very useful in this context.

Let us now consider the tetragonal point group D_{4h} whose character table is given in Tab. A.1. Introduce the character vectors:¹

$$\vec{\chi}_{\mathcal{M}} = (\chi_{\mathcal{M}}(E), \chi_{\mathcal{M}}(C_4), \chi_{\mathcal{M}}(C_2), \chi_{\mathcal{M}}(C'_2), \chi_{\mathcal{M}}(C''_2), \chi_{\mathcal{M}}(P)). \quad (\text{A.9})$$

By employing the character table, one can now easily find the irrep decompositions of direct products, like for instance:

$$\vec{\chi}_{A_{2g} \otimes B_{1u}} = (1, -1, 1, -1, 1, -1) = \vec{\chi}_{B_{2u}}, \quad (\text{A.10})$$

$$\vec{\chi}_{E_g \otimes B_{2g}} = (2, 0, -2, 0, 0, 2) = \vec{\chi}_{E_g}, \quad (\text{A.11})$$

$$\vec{\chi}_{E_g \otimes E_u} = (4, 0, 4, 0, 0, -4) = \vec{\chi}_{A_{1u}} + \vec{\chi}_{A_{2u}} + \vec{\chi}_{B_{1u}} + \vec{\chi}_{B_{2u}}, \quad (\text{A.12})$$

and so forth. In the case of 1D irreps, the above completely answers what we get after a direct product. In the case of 2D irreps, however, special care needs to be taken to ensure that the 2D vectors transform under the same 2D irrep matrices:

$$\mathcal{M}_E(C_{4z}) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \mathcal{M}_E(C_{2x}) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \mathcal{M}_E(C_{2d+}) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (\text{A.13})$$

Regarding parity, because it commutes with everything, in the direct product one can treat it separately from the rotational part D_4 of D_{4h} . After going through all the possible irreps of the D_{4h} point group, one obtains the irrep product table A.2, which was previously also provided in Ref. [24]. Let us note that in the case of $E(\mathbf{v}) \otimes E(\mathbf{u})$, it is convenient to write the result in terms of Pauli matrices:

$$\begin{aligned} \mathbf{v}^\top \sigma_0 \mathbf{u} &\in A_1, & \mathbf{v}^\top \sigma_x \mathbf{u} &\in B_2, \\ \mathbf{v}^\top \sigma_y \mathbf{u} &\in A_2, & \mathbf{v}^\top \sigma_z \mathbf{u} &\in B_1. \end{aligned} \quad (\text{A.14})$$

¹Improper rotations and reflections need not be included in the vector because parity commutes with everything.

Table A.2: **The product table(s) for irreducible representations of the tetragonal point group** $D_{4h} = \{1, P\} \times D_4$ [24].

The upper table is the product table for $\{1, P\}$, which has an even (g) and odd (u) irrep, while the lower table is the product table for D_4 . Both tables are symmetric in the sense that $\zeta(\mathbf{v}) \otimes \xi(\mathbf{u}) = \xi(\mathbf{u}) \otimes \zeta(\mathbf{v})$ for irreps ζ, ξ . For D_4 , notice how the products between 1D irreps have the structure of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ group, with the first $\mathbb{Z}_2 = \{A, B\}$ and the second one corresponding to the subscripts $\{1, 2\}$. In the case of the 2D irrep E , we have ensured that the two components always transform under the same set of matrices of Eq. (A.13). In particular, the ordering is important since $E(u_1|u_2)$ and $E(u_2|u_1)$ imply different transformation rules for $\mathbf{u} = (u_1, u_2)$. Thus, when multiplied with a 1D irrep, the vector components sometimes need to be permuted or negated to ensure that the transformation matrices stay the same.

\otimes	g	u
g	g	u
u	u	g

\otimes	$A_1(u)$	$A_2(u)$	$B_1(u)$	$B_2(u)$	$E(u_1 u_2)$
$A_1(v)$	$A_1(vu)$	$A_2(vu)$	$B_1(vu)$	$B_2(vu)$	$E(vu_1 vu_2)$
$A_2(v)$	$A_2(vu)$	$A_1(vu)$	$B_2(vu)$	$B_1(vu)$	$E(vu_2 -vu_1)$
$B_1(v)$	$B_1(vu)$	$B_2(vu)$	$A_1(vu)$	$A_2(vu)$	$E(vu_1 -vu_2)$
$B_2(v)$	$B_2(vu)$	$B_1(vu)$	$A_2(vu)$	$A_1(vu)$	$E(vu_2 vu_1)$
$E(v_1 v_2)$	$E(v_1u v_2u)$	$E(v_2u -v_1u)$	$E(v_1u -v_2u)$	$E(v_2u v_1u)$	$A_1(v_1u_1 + v_2u_2)$ $A_2(v_1u_2 - v_2u_1)$ $B_1(v_1u_1 - v_2u_2)$ $B_2(v_1u_2 + v_2u_1)$

Notation and Conventions

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Basic quantities:

T	temperature
T_c	superconducting transition temperature
μ	chemical potential
p	hole doping

List of Abbreviations

AF	antiferromagnet/antiferromagnetic/antiferromagnetism
ARPES	angle-resolved photoemission spectroscopy
BCS	Bardeen-Cooper-Schrieffer
BZ	Brillouin zone
CDW	charge-density wave

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List of Publications

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Acknowledgments

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