13 Group-Theoretical Classification of Superconducting States

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1 Introduction

Superconductivity is understood as a condensation of pairs of electrons. As such, it is a rather subtle case of spontaneous symmetry breaking involving *off-diagonal long range order* (ODLRO), and is usually described in terms of spontaneously broken electromagnetic $U(1)$ gauge symmetry [1]. This chapter is about superconductors that break other symmetries, specifically point-group symmetries, in addition to $U(1)$ gauge symmetry. For lack of space and time, we focus on the theoretical classification of such states, not on experimental evidence or phenomenology.

1.1 Notation

Let us first establish the notation. We consider a crystalline solid with N_b "active" electron bands. Electron states are usually described in the Bloch-band basis, with wave functions $\varphi_{\mathbf{k},a}(\mathbf{x})$ for band a and wave vector $\mathbf{k}$, or in a Wannier-orbital basis, with wave functions $w_m(\mathbf{x}-\mathbf{r})$ for the Wannier orbital $m = 1,\ldots,N_b$ centered at the lattice site $\mathbf{r}$. We are used to the latter in the context of strongly correlated electrons. In second-quantized language, we express various physical observables in terms of creation and annihilation operators. In particular, the operator $\Psi_\sigma(\mathbf{x})$ annihilates an electron of spin projection σ ($\sigma = \uparrow,\downarrow$) at the continuous position $\mathbf{x}$ and obeys the anticommutation relations

$$\bigl\{\Psi_\sigma(\mathbf{x}),\, \Psi^\dagger_{\sigma'}(\mathbf{x}')\bigr\} = \delta_{\sigma\sigma'}\,\delta(\mathbf{x}-\mathbf{x}') \qquad \bigl\{\Psi_\sigma(\mathbf{x}),\, \Psi_{\sigma'}(\mathbf{x}')\bigr\} = 0\,. \tag{1}$$

The operator $\Psi_\sigma(\mathbf{x})$ can be expressed in the Bloch basis as

$$\Psi_\sigma(\mathbf{x}) = \sum_{\mathbf{k},a,\sigma} d_{a,\sigma}(\mathbf{k})\,\varphi_{\mathbf{k},a}(\mathbf{x}) \quad \text{where} \quad \{d_{a,\sigma}(\mathbf{k}),\, d^\dagger_{b,\sigma'}(\mathbf{k}')\} = (2\pi)^3\delta(\mathbf{k}-\mathbf{k}')\,\delta_{a,b}\,\delta_{\sigma,\sigma'}\,, \tag{2}$$

or in the Wannier basis as

$$\Psi_\sigma(\mathbf{x}) = \sum_{\mathbf{r},m,\sigma} c_{\mathbf{r},m,\sigma}\,w_{m,\sigma}(\mathbf{x}-\mathbf{r}) \quad \text{where} \quad \{c_{\mathbf{r},m,\sigma},\, c^\dagger_{\mathbf{r}',m',\sigma'}\} = \delta_{\mathbf{r},\mathbf{r}'}\,\delta_{m,m'}\,\delta_{\sigma,\sigma'}\,. \tag{3}$$

A non-interacting Hamiltonian for the free propagation of such electrons takes, in the Wannier basis, the general form

$$H_0 = \sum_{\mathbf{r},\mathbf{r}',m,m',\sigma} t^{m,m'}_{\mathbf{r},\mathbf{r}'}\,c^\dagger_{\mathbf{r},m,\sigma}\,c_{\mathbf{r}',m',\sigma} \tag{4}$$

(we ignore the spin-orbit (SO) interaction for the moment). If $c_{m,\sigma}(\mathbf{k})$ is the Fourier transform of $c_{\mathbf{r},m,\sigma}$, the above Hamiltonian may be written in a simpler form, diagonal in $\mathbf{k}$ because of translation invariance on the lattice

$$H_0 = \sum_{\mathbf{k},m,m',\sigma} t^{m,m'}(\mathbf{k})\,c^\dagger_{m,\sigma}(\mathbf{k})\,c_{m',\sigma}(\mathbf{k}) \tag{5}$$

(we will call this description the *orbital basis*). Finally, the $\mathbf{k}$-dependent $N_b\times N_b$ matrix $t^{m,m'}(\mathbf{k})$ may be diagonalized by a unitary matrix $V_{a,m}(\mathbf{k})$, which brings us to the annihilation operator

$d_{\mathbf{k},a}(\mathbf{k})$ in the Bloch basis

$$d_{a,\sigma}(\mathbf{k}) = \sum_m V_{a,m}(\mathbf{k})\, c_{m,\sigma}(\mathbf{k}) \tag{6}$$

in terms of which the non-interacting Hamiltonian becomes completely diagonal

$$H_0 = \sum_{\mathbf{k},a,\sigma} \varepsilon_a(\mathbf{k})\; d^\dagger_{a,\sigma}(\mathbf{k})\, d_{a,\sigma}(\mathbf{k})\;. \tag{7}$$

In practice, band structure calculations provide us with the band energies $\varepsilon_a(\mathbf{k})$ and the wave functions $\varphi_{\mathbf{k},a}(\mathbf{x})$, from which Wannier functions can be obtained with some degree of arbitrariness, although a maximal localization principle can be followed [2]. Alternatively, the Wannier basis can be the starting point, using a tight-binding approximation.

1.2 Pairing

The fundamental object of superconductivity is a pair of electrons, or Cooper pair. A generic annihilation operator for a Cooper pair takes the following form, in a translation invariant system[1]

$$\hat{\Delta} = \int d^3\mathbf{r}\; d^3\mathbf{r}'\; \Delta_{\sigma\sigma'}(\mathbf{r}-\mathbf{r}')\; \Psi_\sigma(\mathbf{r})\, \Psi_{\sigma'}(\mathbf{r}')\;. \tag{8}$$

Because of the Pauli principle, i.e., anticommutation relations (1), we can impose an antisymmetry condition on the amplitude

$$\Delta_{\sigma\sigma'}(\mathbf{r}-\mathbf{r}') = -\Delta_{\sigma'\sigma}(\mathbf{r}'-\mathbf{r})\;. \tag{9}$$

In the Bloch basis, this pairing operator and the antisymmetry condition are expressed as

$$\hat{\Delta} = \sum_{\mathbf{k},a,b,\sigma,\sigma'} \Delta_{a\sigma,b\sigma'}(\mathbf{k})\; d_{a\sigma}(\mathbf{k})\, d_{b\sigma'}(-\mathbf{k}) \qquad \Delta_{a\sigma,b\sigma'}(\mathbf{k}) = -\Delta_{b\sigma',a\sigma}(-\mathbf{k})\,. \tag{10}$$

Likewise, in the Wannier basis,

$$\hat{\Delta} = \sum_{\mathbf{r},\mathbf{r}',m,m',\sigma,\sigma'} \Delta_{\mathbf{r}m\sigma,\mathbf{r}'m'\sigma'}\; c_{\mathbf{r}m\sigma}\, c_{\mathbf{r}'m'\sigma'} \qquad \Delta_{\mathbf{r}m\sigma,\mathbf{r}'m'\sigma'} = -\Delta_{\mathbf{r}'m'\sigma',\mathbf{r}m\sigma} \tag{11}$$

and, in the orbital basis,

$$\hat{\Delta} = \sum_{\mathbf{k},m,m',\sigma,\sigma'} \Delta_{m\sigma,m'\sigma'}(\mathbf{k})\; c_{m\sigma}(\mathbf{k})\, c_{m'\sigma'}(-\mathbf{k}) \qquad \Delta_{m\sigma,m'\sigma'}(\mathbf{k}) = -\Delta_{m'\sigma',m\sigma}(-\mathbf{k})\,. \tag{12}$$

A general order parameter function (or pairing function) can be expressed as a linear combination of basis functions. We can use a basis made of products of $\mathbf{k}$-dependent, orbital-dependent and spin-dependent factors. In the orbital basis, this takes the form

$$\Delta_{m,\sigma;m',\sigma'}(\mathbf{k}) = \sum_{\alpha\beta\gamma} \psi_{\alpha\beta\gamma}\, f^\alpha(\mathbf{k})\, O^\beta_{mm'}\, S^\gamma_{\sigma\sigma'}\;. \tag{13}$$

[1] We ignore here the possibility of *pairing waves*, i.e., of Cooper pairs having a finite momentum. The Fulde-Ferrell-Larkin-Ovchinnikov state in an example where such pairing may occur. For another example, see Ref. [3].

where the amplitudes $\psi_{\alpha\beta\gamma}$ determine the precise form of pairing, given a suitable choice for the basis functions $f^\alpha(\mathbf{k})$ (momentum space), $O^\beta_{mm'}$ (orbital space) and $S^\gamma_{\sigma\sigma'}$ (spin space). In the Bloch basis, the expansion would be similar

$$\Delta_{a,\sigma;b,\sigma'}(\mathbf{k}) = \sum_{\alpha\beta\gamma} \chi_{\alpha\beta\gamma}\, f^\alpha(\mathbf{k})\, B^\beta_{ab}(\mathbf{k})\, S^\gamma_{\sigma\sigma'} \ , \tag{14}$$

with a different set of amplitudes $\chi_{\alpha\beta\gamma}$, and $\mathbf{k}$-dependent basis functions $B^\beta_{ab}(\mathbf{k})$ in "band space". The reason the basis functions $O^\beta_{mm'}$ do not depend on $\mathbf{k}$ is that Wannier functions can be chosen to have a clear "orbital character" in space, like atomic orbitals, which transform in a well-defined way under rotations and reflections (Section 4.2 will provide an example of this). Consequently, the band basis functions B^β_{ab} must depend on $\mathbf{k}$; this makes the discussion of inter-band superconductivity more complex in the Bloch basis than in the orbital basis.
Each of the spatial, orbital (or band) and spin parts can be either symmetric or antisymmetric under the exchange of quantum numbers, but he overall combination must be antisymmetric. For instance, in the absence of SO coupling, spin is conserved and pairing occurs either in the singlet (spin 0) channel or in the triplet (spin 1) channel. In the case of a single band, the spatial part $f(\mathbf{k})$ must then be even ($f(-\mathbf{k}) = f(\mathbf{k})$) for singlet pairing, and odd ($f(-\mathbf{k}) = -f(\mathbf{k})$) for triplet pairing. This remains so in the case of intra-orbital (or intra-band) pairing, i.e., when $O^\beta_{mm'} = 0$ for $m \neq m'$, but inter-orbital pairing brings other possibilities, and spin-orbit interactions complicate the matter further.

1.2.1 Spin part

The conventional way to describe the spin part is as follows

$$S_{\sigma\sigma'} = d_\gamma(\hat{\mathbf{d}}_\gamma)_{\sigma\sigma'} \qquad\qquad \hat{\mathbf{d}}_\gamma = i(\tau_\gamma\tau_2) \ , \tag{15}$$

where the set of Pauli matrices $\tau_{1,2,3}$ is augmented by the identity matrix τ_0. The three components $\gamma = 1, 2, 3$ form the symmetric, triplet part of the pairing function, whereas the antisymmetric, singlet part is represented by the component $\gamma = 0$.
Under a rotation in spin space, the 3-vector (d_x, d_y, d_z) (or (d_1, d_2, d_3)) transforms as a pseudo-vector (i.e., invariant under spatial inversion) and constitutes the triplet component, whereas d_0 behaves like a pseudo-scalar (it changes signs under inversion) and constitutes the singlet component. In the absence of SO coupling, the system being invariant under spin rotations, the pairing function fully factorizes into a spin part and the rest. In other words, all terms in the expansion (13) have the same spin part, and the pairing state can be characterized by a fixed vector (d_x, d_y, d_z) (triplet pairing) or by d_0 (singlet pairing).

1.2.2 Spatial part

The spatial part $f(\mathbf{k})$ of the pairing function could equally well be described in real space

$$f(\mathbf{k}) = \sum_{\mathbf{r}} f_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} \tag{16}$$

where $f_{\mathbf{r}}$ is, so to speak, the pairing amplitude for electrons separated by a lattice vector $\mathbf{r}$. The spatial extent of the Cooper pair is called the *coherence length*, denoted ξ. This roughly means that $f_{\mathbf{r}}$ typically drops exponentially as a function of $\mathbf{r}$ with a characteristic length ξ. For short coherence lengths, $f_{\mathbf{r}}$ is dominated by the smallest values of $\mathbf{r}$: on-site ($\mathbf{r}$=$\mathbf{0}$) and nearest-neighbor amplitudes. Pure on-site pairing means $f_{\mathbf{r}} = \delta_{\mathbf{r},\mathbf{0}}$ and therefore a $\mathbf{k}$-independent amplitude. The celebrated d-wave pairing on a square lattice with unit lattice vectors $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ means $f_{\pm\hat{\mathbf{x}}} = -f_{\pm\hat{\mathbf{y}}}$, all other amplitudes being zero, and therefore $f(\mathbf{k}) = \cos k_x - \cos k_y$.

1.3 Mean-field approximation and nodal lines

In the mean-field approximation, a constant and uniform pairing field is assumed to pervade the system. The effective Hamiltonian for singlet superconductivity then takes the following form, in the Bloch basis

$$H_0 = \sum_{\mathbf{k},a,\sigma} \varepsilon_a(\mathbf{k})\; d^\dagger_{a,\sigma}(\mathbf{k})\, d_{a,\sigma}(\mathbf{k}) + \sum_{\mathbf{k},a,b} \Delta_{ab}(\mathbf{k}) \big[d_{a\uparrow}(\mathbf{k})\, d_{b\downarrow}(-\mathbf{k}) - d_{a\downarrow}(\mathbf{k})\, d_{b\uparrow}(-\mathbf{k}) \big] \tag{17}$$

(We assume that the chemical potential μ is included in the dispersion relation $\varepsilon_a(\mathbf{k})$ as an additive constant.) In order to diagonalize this Hamiltonian, one introduces an extended array of annihilation operators[2]

$$\Psi(\mathbf{k}) = \big(d_{1\uparrow}(\mathbf{k}), \ldots, d_{N_b\uparrow}(\mathbf{k}), d^\dagger_{1\downarrow}(-\mathbf{k}), \ldots, d^\dagger_{N_b\downarrow}(-\mathbf{k}) \big)\,. \tag{18}$$

The second half of the array $\Psi(\mathbf{k})$ is basically the particle-hole transformation of the first half; this procedure is attributed to Nambu. Because we are dealing with fermions, the components of $\Psi(\mathbf{k})$ still obey anticommutation relations and we can treat them as *bona fide* annihilation operators. One can then express H_0 as

$$H_0 = \sum_{\mathbf{k}} \Psi^\dagger(\mathbf{k}) \mathcal{H}(\mathbf{k}) \Psi(\mathbf{k}) \tag{19}$$

where $\mathcal{H}(\mathbf{k})$ is a $2N_b \times 2N_b$ matrix with the following block structure:

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} \boldsymbol{\epsilon}(\mathbf{k}) & \boldsymbol{\Delta}^\dagger(\mathbf{k}) \\ \boldsymbol{\Delta}(\mathbf{k}) & -\boldsymbol{\epsilon}(-\mathbf{k}) \end{pmatrix} \tag{20}$$

where $\boldsymbol{\epsilon}(\mathbf{k})$ is the diagonal matrix with elements $\varepsilon_a(\mathbf{k})$ and $\boldsymbol{\Delta}(\mathbf{k})$ is the matrix of band components $\Delta_{ab}(\mathbf{k})$.

To complete the analysis, we need to diagonalize the Hermitian matrix $\mathcal{H}(\mathbf{k})$ via a *Bogoliubov transformation*. Because of the particular structure of the matrix $\mathcal{H}(\mathbf{k})$, its eigenvalues come in pairs of opposite signs and the ground state (the superconducting condensate) is obtained by

[2] This particular form works well when the $\mathbf{d}$-vector is d_0 or d_z. In other cases, or when spin is not conserved, one must proceed to a full Nambu doubling of the degrees of freedom,
i.e., $\Psi(\mathbf{k}) = \big(d_{1\uparrow}(\mathbf{k}), \ldots, d_{N_b\uparrow}(\mathbf{k}), d_{1\downarrow}(\mathbf{k}), \ldots, d_{N_b\downarrow}(\mathbf{k}), d^\dagger_{1\downarrow}(-\mathbf{k}), \ldots, d^\dagger_{N_b\downarrow}(-\mathbf{k}), d^\dagger_{1\uparrow}(-\mathbf{k}), \ldots, d^\dagger_{N_b\uparrow}(-\mathbf{k}) \big)$.

filling all the negative energy levels. The resulting new set of annihilation operators annihilate quasiparticles on top of the superconducting ground state.
As a simple example, let us consider a one-band model ($N_b = 1$). $\boldsymbol{\epsilon} \to \epsilon$ and $\boldsymbol{\Delta} \to \Delta$ are then scalar functions and the eigenvalues of Hamiltonian (20) are then easily computed to be

$$\xi(\mathbf{k}) = \pm\sqrt{\varepsilon^2(\mathbf{k}) + \Delta^2(\mathbf{k})} \tag{21}$$

Recall that the chemical potential is included in the function $\varepsilon(\mathbf{k})$, so that the Fermi surface is defined by the condition $\varepsilon(\mathbf{k}) = 0$. Low-energy quasiparticles will exist on top of the condensate if $\xi(\mathbf{k}) = 0$ for some values of $\mathbf{k}$ that we call *nodes*. In this simple, one-band case, nodes exist when both scalar functions $\varepsilon(\mathbf{k})$ and $\Delta(\mathbf{k})$ vanish. For instance, in the well-known case of d-wave superconductivity on a square lattice, $\Delta(\mathbf{k}) \propto \cos k_x - \cos k_y$ and the nodes are located along the diagonals of the Brillouin zone : $k_x = \pm k_y$. When more than one band is present, complications occur (see Sect. 4.3 below).

2 Elements of group theory

2.1 Groups

Since group theory is not necessarily familiar to all, we will review the basics in this section, with en emphasis on finite groups.[3]
A group G is a set $\{a, b, c, \ldots\}$ endowed with a multiplication law satisfying the following constraints:

1. Group multiplication is associative: $(ab)c = a(bc)$.
2. There is a neutral element e such that $ea = ae = a\,, \forall a \in G$.
3. Each element a has an inverse a^{-1} such that $aa^{-1} = a^{-1}a = e$.

It is implicit that if $a, b \in G$, then $ab \in G$ (closure under the group multiplication).
These rules are obeyed by the set of all nonsingular square matrices of order n, called $GL(n)$. A *subgroup* H of G is a subset of G that is also a group under the same multiplication law, i.e., that is closed under group multiplication. For instance, the group $O(n)$ is the subgroup of $GL(n)$ made of orthogonal matrices. A group is *continuous* if its elements form a topological space, i.e., a space with the notion of continuity. In particular, a *Lie group* is also a differentiable manifold ($O(n)$ is a Lie group). By contrast, a *discrete group* has well-separated elements, and a *finite group* has a finite number of such elements. In general group multiplication is not commutative; when it is, the group is said to be *Abelian*, otherwise it is *nonabelian*. A subset of elements of G are called *generators* if all elements of the group (with the exception of e) may be obtained by repeated products within the subset.
The point groups of solid-state physics are finite subgroups of $O(n)$, and as such are sets of rotations and reflections closed under repeated application. We will often refer to the elements

[3] There is a large selection of textbooks on group theory. Let us point out the classic Hamermesh text [4], as well as the more recent "nutshell" text by A. Zee [5].

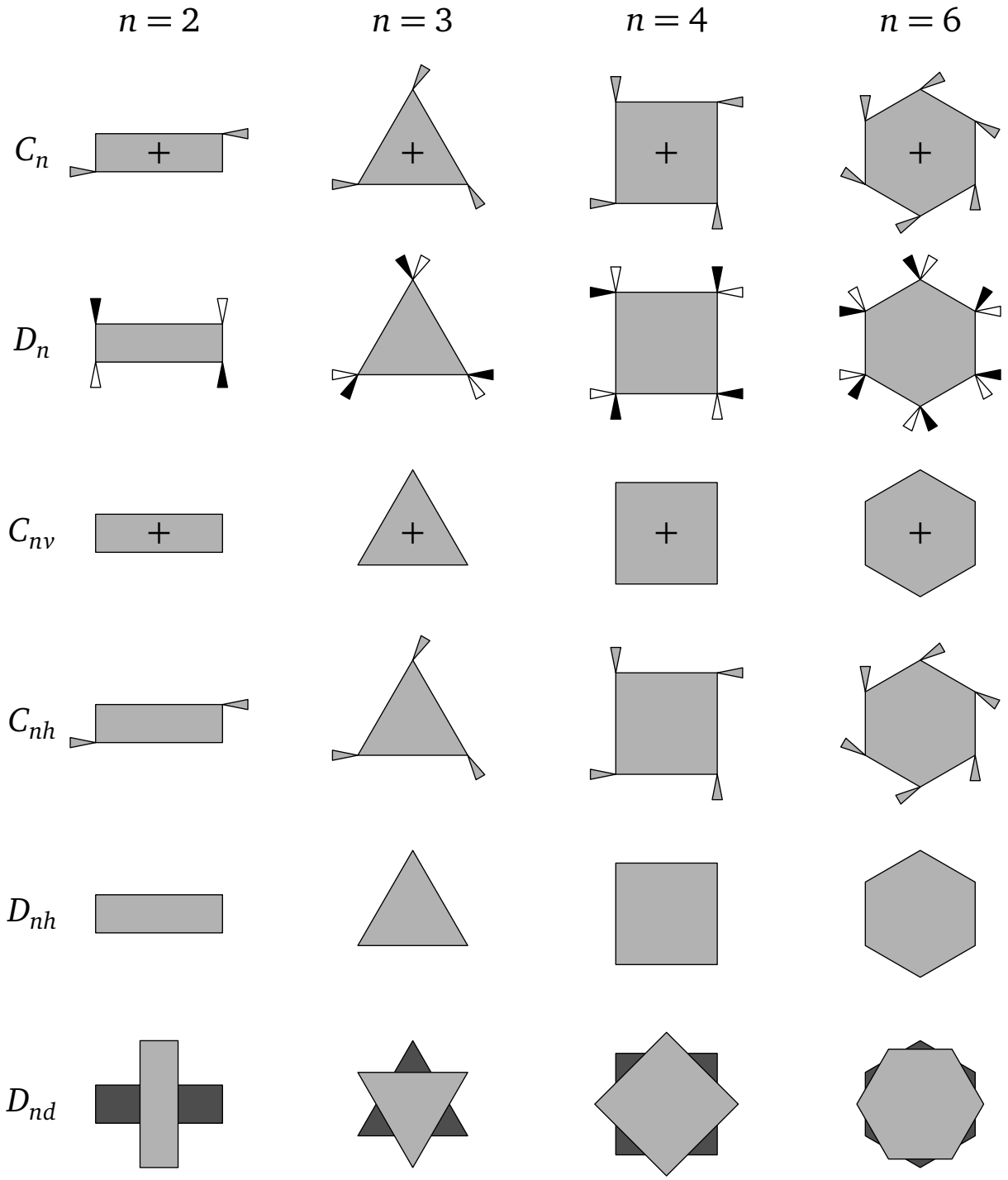


Fig. 1: *Graphical definition of the most common point groups. The group elements are those that leave each figure unchanged. Decorations added to vertices are geometrical features that rest on the plane of the page (gray), stick out of it (white) or into it (black). The darker colored objects are underneath the lighter ones. Objects marked with a + sign have a top face distinct from their bottom face and thus have no mirror symmetry about the plane or rotation axes lying in the plane.*

of these groups as *transformations*, as they can be viewed as acting on an object or physical configuration. The most common point groups can be defined as transformations on simple objects as illustrated on Fig. 1:[4]

1. C_n (cyclic group): the group elements are rotations by $2\pi/n$ about the z axis (perpendicular to the plane).
2. D_n (dihedral group): in addition to the rotations of C_n, the group contains n rotations of π about n axes lying on the xy plane.
3. C_{nv} (pyramidal group): in addition to the rotations of C_n, the group contains n reflections across n mirror planes perpendicular to the xy plane.
4. C_{nh} (reflection group): in addition to the rotations of C_n, the group contains a reflection across the xy plane.
5. D_{nh} (prismatic group): in addition to the $2n$ rotations of D_n, the group contains a reflection across the xy plane.
6. D_{nd} (antiprismatic group): Similar to D_{nh}, except that the n π-rotation axes lying on the xy plane are not the intersection of the xy plane with the n mirror planes perpendicular to the xy plane. Rather, these axes are alternating with these intersections.

2.2 Representations

In general, we are dealing with *group representations*, i.e., realizations of the group elements in terms of d-dimensional matrices acting on some space (that space V is called the *module* of the representation). A group element a is represented by a matrix $R(a)$ and that correspondence is a *homomorphism* with respect to the group operation: $R(ab) = R(a)R(b)$. Two representations R and R' are said to be *equivalent* if they are related by a change of basis, i.e., $R(a) = SR'(a)S^{-1}, \forall a \in G$. For a finite group, it can be shown that any representation is equivalent to a unitary representation, i.e., a representation made of unitary (or orthogonal) matrices, such that $R(a^{-1}) = R^{-1}(a) = R^{\dagger}(a)$. A simple example of a representation for the group C_{4v} is given in Table 1.

A representation is said to be *reducible* if a basis exists in the module V of the representation such that all elements $R(a)$ have the same block-diagonal structure. This means that the module can be seen as the direct sum of two submodules: $V = V_1 \oplus V_2$, each of $V_{1,2}$ being the support for a representation in its own right. In other words, the two submodules are not mixed with one another when acted upon by the group elements. Otherwise, the representation is said to be *irreducible*. One of the common tasks of group theory is the reduction of representations in terms of *irreps* (as irreducible representations are often called). The representation shown in Table 1 happens to be irreducible.

[4] In a crystalline solid, one should in principle consider the full *space group*, which contains translations as well as rotations and reflections. But translation invariance amounts to say that the gap function depends on a single wave vector $\mathbf{k}$, and the presence of the lattice implies that it should be unchanged when replacing $\mathbf{k}$ by $\mathbf{k} + \mathbf{Q}$, where $\mathbf{Q}$ is an element of the reciprocal lattice.

Table 1: *A simple example of group representation for C_{4v}: the matrices act on the coordinates (x, y). C_n is a rotation by $2\pi/n$ in the x-y plane. σ_x, σ_y, σ_d and $\sigma_{d'}$ are reflections across the planes $x = 0$, $y = 0$, $x = -y$ and $x = y$, respectively.*

g	$R(g)$	g	$R(g)$	g	$R(g)$	g	$R(g)$
e	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	C_4	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	C_4^{-1}	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	C_2	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$
σ_x	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	σ_y	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	σ_d	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\sigma_{d'}$	$\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$

A capital result of group theory are *Schur's lemmata*:

1. If R and R' are two irreps of different dimensions $d \neq d'$, then no nonzero rectangular matrix A exists such that $R(a)A = AR'(a)\ \ \forall a \in G$.
2. If R and R' are two irreps of the same dimension $d = d'$ and if a square matrix A exists such that $R(a)A = AR'(a)\ \ \forall a \in G$, then the two representations are equivalent.

The consequence of these two lemmata is the following. Consider a module V upon which a reducible representation acts. Then $V = V_1 \oplus V_2$ is a direct sum, and so is each element of the representation: $R(a) = R_1(a) \oplus R_2(a)$. Let H be a matrix acting on V that commutes with all the group elements, i.e., $HR(a) = R(a)H$. If the representations R_1 and R_2 are not equivalent, then H is necessarily block diagonal too, i.e., has no matrix elements between V_1 and V_2. Typically, in quantum mechanics, H is a Hamiltonian acting on a Hilbert space and G is a group of transformations that commute with H, i.e., that leave the Hamiltonian invariant. The construction of irreps then allows us to consider smaller spaces (the blocks) that are not mixed with one another under time evolution. Said otherwise, energy eigenstates and eigenvalues can be classified according to the irreps of the symmetry group of the problem.

2.3 Character tables

An important tool in identifying irreps of finite groups is the notion of *character*. Let us start by defining *conjugacy classes*. Two elements a and b of a group G are *conjugate* to one another if there is another element c such that $a = cbc^{-1}$. Intuitively, this means that the two transformations a and b are of the "same type", as c can be seen as a change of basis (or point of view), after which the two transformations a and b are equivalent. For instance, in the group C_{4v}, $a = \sigma_x$ and $b = \sigma_y$ are related by the rotation $c = C_4$: they are conjugate. Evidently, if a is conjugate to b and b is conjugate to a third element c, then a is also conjugate to c: conjugacy is an equivalence relation and therefore the group G can be split into separate *conjugacy classes*. Obviously, the identity e is a conjugacy class by itself. In C_{4v}, the two mirror reflections collectively denoted σ_v (σ_x and σ_y) form a class, as do the two reflections σ_d and $\sigma_{d'}$ and the two rotations C_4 and C_4^{-1}; finally, the single rotation by π (C_2) is a class by itself. Thus, C_{4v} has 5 conjugacy classes and 8 elements.

Table 2: *Character table of C_{4v}, with a list of the simplest (i.e., lowest degree) basis functions. The basis functions of the two-dimensional representation E form a doublet, written here and elsewhere in this chapter within square brackets $[\cdots,\cdots]$. The last column shows the gap basis functions derived in Sect. 3.1.*

	e	$2C_4$	C_2	$\sigma_{x,y}$	$\sigma_{d,d'}$	basis functions	gap functions
A_1	1	1	1	1	1	1	1
A_2	1	1	1	-1	-1	$\mathcal{R}_z\ ,\ xy(x^2-y^2)$	$\sin k_x\ \sin k_y(\cos k_x-\cos k_y)$
B_1	1	-1	1	1	-1	x^2-y^2	$\cos k_x-\cos k_y$
B_2	1	-1	1	-1	1	xy	$\sin k_x\ \sin k_y$
E	2	0	-2	0	0	$[\mathcal{R}_x,\mathcal{R}_y]\ ,\ [x,y]$	$[\sin k_x,\sin k_y]$

The *character* $\chi(a)$ of an element a in a representation R is the trace of that matrix: $\chi(a) = \operatorname{tr} R(a)$. Because of the cyclic property of the trace, two conjugate elements have the same character in a given representation, and therefore characters are properties of conjugacy classes, not of individual elements. We can therefore envisage a matrix-like table, called a *character table*, where the different irreps are laid out in rows and the different conjugacy classes in columns, each cell containing the character $\chi_i^{(\mu)}$ for the conjugacy class i within the irrep μ. See, for instance, Table 2 for C_{4v}, Table 3 for D_{4h} and Table 4 for C_{6v}. Note that the dimension of each irreducible representation is naturally given by the character of the identity class e.
Schur's lemma can be used to demonstrate the following orthogonality relation

$$\sum_i^K \frac{g_i}{g}\,\chi_i^{(\nu)*}\chi_i^{(\mu)} = \delta_{\mu\nu}\ , \tag{22}$$

where g stands for the number of elements of the group G, g_i is the number of elements in conjugacy class i, and K is the number of conjugacy classes. This relation states that the different rows of the character table are orthogonal (if weighted by g_i). This implies that there cannot be more than K rows in the table, as the rows are vectors of dimension K. Indeed, it can be shown that the number of non-equivalent irreps is precisely equal to K and that

$$\sum_\mu^K d_\mu^2 = g \tag{23}$$

where d_μ is the dimension of irrep μ. Finally, the orthogonality of the rows of the character table also applies to its columns:

$$\sum_\mu^K \frac{g_i}{g}\,\chi_i^{(\mu)*}\chi_j^{(\mu)} = \delta_{ij}\ . \tag{24}$$

These powerful orthogonality relations allow us to decompose any reducible representation R into a direct sum of irreps. Indeed, a general reducible representation can in principle be

Table 3: *Character table of D_{4h}, with a list of the lowest degree basis functions.*

	e	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_z	$\sigma_{x,y}$	$\sigma_{d,d'}$	basis functions
A_{1g}	1	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	−1	−1	1	1	1	−1	−1	$\mathcal{R}_z\ ,\ xy(x^2-y^2)$
B_{1g}	1	−1	1	1	−1	1	−1	1	1	−1	x^2-y^2
B_{2g}	1	−1	1	−1	1	1	−1	1	−1	1	xy
E_g	2	0	−2	0	0	2	0	−2	0	0	$[\mathcal{R}_x, \mathcal{R}_y]\ ,\ z[x,y]$
A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1	$xyz(x^2-y^2)$
A_{2u}	1	1	1	−1	−1	−1	−1	−1	1	1	z
B_{1u}	1	−1	1	1	−1	−1	1	−1	−1	1	xyz
B_{2u}	1	−1	1	−1	1	−1	1	−1	1	−1	$z(x^2-y^2)$
E_u	2	0	−2	0	0	−2	0	2	0	0	$[x,y]$

expressed as

$$R = \bigoplus_{\mu}^{K} a_\mu R^{(\mu)}\,. \tag{25}$$

The a priori unknown integer a_μ (the multiplicity of $R^{(\mu)}$ in R) can be determined by use of the orthogonality relation (22), using the known characters χ_i of the reducible representation R

$$a_\mu = \sum_{i}^{K} \frac{g_i}{g}\,\chi_i^{(\mu)*}\chi_i\,. \tag{26}$$

The reducible representation R acts on a module V which, likewise, is a direct sum of irreducible modules

$$V = \bigoplus_{\mu}^{K} V^{(\mu)}. \tag{27}$$

A vector ψ belonging to the module V will be affected by the transformation $a \in G$ as $\psi \to R(a)\psi$. It can be shown that the components of ψ along the submodule $V^{(\mu)}$ associated to the irrep μ can be obtained by applying on ψ the following *projection operator*

$$P^{(\mu)} = \sum_{a} \frac{d_\mu}{g}\,\chi^{(\mu)*}(a)R(a) \tag{28}$$

where $\chi^{(\mu)}(a)$ is the character of element a in representation μ. In other words, the vector $P^{(\mu)}\psi$ belongs to the submodule $V^{(\mu)}$ and, when acted upon by any transformation $a \in G$, will stay in this submodule. Projection operators are exceedingly useful in constructing basis functions (or, in superconductivity applications, gap functions) from tensor products.

2.4 Example: The D_{4h} character table

Let us illustrate the ideas behind character tables with a more complex example than C_{4v}: The point group D_{4h}. This group has the following $K = 10$ conjugacy classes:

1. The identity e
2. Two rotations C_4, i.e., of angle $\pi/2$, about the z axis.
3. A rotation C_2, i.e., of angle π, about the z axis.
4. Two rotations C_2' (π) about the x and y axes.
5. Two rotations C_2'' (π) about the diagonal axes $x \pm y$.
6. One space inversion i
7. Two pseudo-rotations S_4 of $\pi/4$ (rotations times inversion).
8. A reflection σ_z across the $z = 0$ plane.
9. 2 reflections $\sigma_{x,y}$ across the $x = 0$ and $y = 0$ planes.
10. 2 reflections $\sigma_{d,d'}$ across planes $y = -x$ and $y = x$.

Correspondingly, there are $K = 10$ irreps, divided into two groups: the g-type representations (first five rows on Table 3) that are even under the space inversion i, and the u-type representations, which are odd under i. For each representation, Table 3 gives an example of functions (homogeneous polynomials in x, y, z), or of rotations (R_x, R_y, R_z), that transform under that representation (in general, the elements of $O(n)$ acting on homogeneous polynomials in $\{x, y, z\}$ will produce another homogeneous polynomial of the same degree. Consequently, homogeneous polynomials of a given degree can be arranged into irreps. Likewise, an orthogonal matrix O will act on a rotation matrix $\mathcal{R}$ as $\mathcal{R} \to O\mathcal{R}O^{-1}$ and produce another rotation matrix about a different axis (equivalently, one could express infinitesimal rotations in terms of pseudo-vectors, and the group elements will act on these pseudo-vectors). Rotations therefore transform under the group and can also be arranged into irreps.
Let us go through some of these representations:

- A_{1g} is the trivial representation, of dimension 1. Each group element is represented by the number 1.
- A_{2g}, of dimension 1, is odd under π-rotations C_2' and C_2'', as well as under the reflections $\sigma_{x,y}$ and $\sigma_{d,d'}$. A rotation $\mathcal{R}_z$ about the z axis belongs to this representation; in particular, it changes sign when rotated by π with respect to a horizontal axis, but not when reflected across the xy plane. It also changes sign when reflected across a vertical mirror plane. The quartic polynomial $xy(x^2-y^2)$ behaves the same way; note that xy does not, because it is even under $\sigma_{d,d'}$.
- B_{1g} is odd under the $\pi/2$ rotations C_4, under the π-rotations C_2'' about the diagonals, under the $\pi/2$ pseudo-rotations S_4, and under the diagonal reflections $\sigma_{d,d'}$. It is well represented by the quadratic polynomial x^2-y^2 and by what we commonly call d-wave superconductivity on a square or cubic lattice.
- B_{2g} is similar, except that it is odd under the other set of reflections and $\pi/2$ rotations, as if rotated by 45° compared to B_{1g}. It is represented by the monomial xy and by d-wave superconductivity, this time with a d_{xy} form factor instead of $d_{x^2-y^2}$.

- E_g is a two-dimensional representation, represented by the doublet of pseudo-vectors $[\mathcal{R}_x, \mathcal{R}_y]$, or by the doublet of monomials $[zx, zy]$.
- The u-type representations have the same characters as the g-type representations for proper transformations (the first 5 columns), and opposite characters for the improper transformations (the last 5 columns). Proper transformations have determinant $+1$ and describe actual transformation that a rigid object may undergo, whereas improper transformation have determinant -1 and can always be viewed as a proper transformation times the inversion i.

2.5 Tensor products

Given two representations $R^{(1)}_{ij}(a)$ and $R^{(2)}_{ij}(a)$ of dimensions d_1 and d_2, acting respectively on modules V_1 et V_2, the product representation of dimension $d_1 d_2$ acts on the tensor product module $V_1 \otimes V_2$ and is made of the tensor products of the matrices of the two representations

$$R_{ik,jl}(a) = R^{(1)}_{ij}(a) R^{(2)}_{kl}(a) \text{ or } R(a) = R^{(1)}(a) \otimes R^{(2)}(a)\,. \tag{29}$$

A product representation is in general reducible, even if the two factors are irreducible. Reducing a product representation to its irreducible components is an important problem of group theory. The direct sum

$$R^{(\mu)} \otimes R^{(\nu)} = \bigoplus_{\rho} C^{\rho}_{\mu\nu}\, R^{(\rho)} \tag{30}$$

is called the *Clebsch-Gordan series*. For one-dimensional representations (including all representations of Abelian groups), this series is trivial since it contains a single term. For multidimensional representations, the series can be inferred from the character table, by noting that the character of a product representation is the product of the characters of its factors

$$\chi_i(R^{(\mu)} \otimes R^{(\nu)}) = \chi^{(\mu)}_i \chi^{(\nu)}_i = \sum_{\rho} C^{\rho}_{\mu\nu} \chi^{(\rho)}_i\,. \tag{31}$$

Applying the orthogonality relation (22) to this relation yields

$$C^{\rho}_{\mu\nu} = \sum_{i=1}^{K} \frac{g_i}{g}\, \chi^{*(\rho)}_i \chi^{(\mu)}_i \chi^{(\nu)}_i\,. \tag{32}$$

The states of the product module $V_1 \otimes V_2$ associated with each component of the Clebsch-Gordan series can be obtained by applying the projection operators (28). An example application of projection operators is given in Sect. 3.1.

2.6 Back to superconductivity: The Landau free energy

We will assume that Landau's theory of phase transitions qualitatively describes the superconducting transition as temperature is lowered. This theory assumes that the broken symmetry state is described by an order parameter ψ, which vanishes in the normal state and develops a

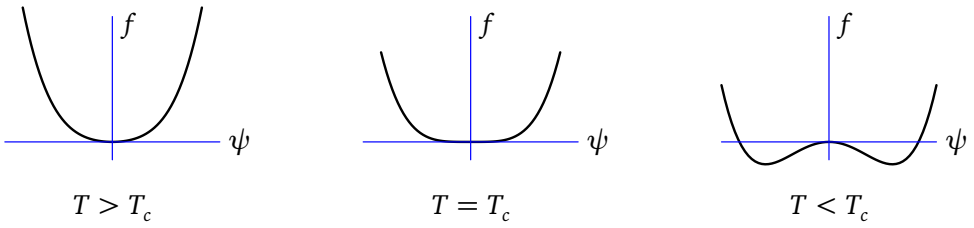


Fig. 2: *Behavior of the Landau free energy functional across a continuous (a.k.a. second order) phase transition.*

nonzero value in the broken symmetry state. It further assumes that a local free energy functional $f[\psi]$ may be defined and that the physical, uniform value of ψ corresponds to a minimum of f (see Fig. 2).

If the precise form of ψ, i.e., the precise pattern of symmetry breaking, is not known, then we may assume that ψ may be decomposed on a basis of possible pairing functions. Going back to Eq. (13), let us combine the three indices α, β, γ into a single index r:

$$\Delta_{m,\sigma;m',\sigma'}(\mathbf{k}) = \sum_r \psi_r \, \Delta^{(r)}_{m,\sigma;m',\sigma'}(\mathbf{k}) \tag{33}$$

The Landau free energy functional is then a power expansion in terms of the coefficients ψ_r:

$$f[\psi] = a_{rs}(T)\psi_r^*\psi_s + b_{rspq}(T)\,\psi_r^*\psi_s^*\psi_p\psi_q + \cdots \tag{34}$$

where the ellipsis stands for gradient- and higher-degree terms, and T is the temperature.

The Landau functional should have the same symmetries as the underlying Hamiltonian. If these symmetries form a group G of transformations, Schur's lemma tells us that organizing the basis functions $\boldsymbol{\Delta}^{(r)}$ according to irreps of G makes the matrix $a(T)$ block-diagonal: $a(T) = \bigoplus_\mu a^{(\mu)}(T)$, i.e., it has no matrix elements between functions belonging to different irreps. Within each representation, the matrix $a^{(\mu)}(T)$ may be diagonalized, and at some point upon lowering T one of its eigenvalues, initially all positive, may change sign, which signals the superconducting phase transition and a minimum of $f[\psi]$ at $\psi \neq 0$. This is going to first occur in one of the representations and will define the symmetry character of the superconducting state.[5]

For this reason it is important to arrange the possible gap functions into irreps of the symmetry group G. It amounts to a classification of possible superconducting states. Of course, a precise physical theory—a microscopic Hamiltonian—is needed in order to determine in which irrep superconductivity actually appears; but this is not the subject of this chapter.

Since the basis functions are products of spin, orbital and spatial factors, the group theoretical analysis can be done on each of these factors separately, followed by suitable tensor products. In the absence of SO coupling, the system is invariant under rotations in spin space; this leads to a clear separation between singlet and triplet gap functions, and only the combined orbital and spatial factors need to be classified according to the point group G.

[5] This is the simplest scenario, but nothing forbids competing minima, and hence additional phase transitions, to appear at lower temperatures.

3 Single-band superconductors

Let us continue our exploration by focusing first on single-band superconductors. In the absence of SO coupling, the classification of gap functions according to the point group is then limited to the spatial part. The exponentials $e^{i\mathbf{k}\cdot\mathbf{r}}$ form a set of basis functions $f^{\mathbf{r}}(\mathbf{k})$ for the spatial part. Under an element g of the point group, $\mathbf{k} \to g\mathbf{k}$ and $e^{i\mathbf{k}\cdot\mathbf{r}}$ is mapped into $e^{ig\mathbf{k}\cdot\mathbf{r}} = e^{i\mathbf{k}\cdot(g^{-1}\mathbf{r})}$. Given a lattice vector $\mathbf{r}$, the set of functions labeled by $S = \{g\mathbf{r}\},\ g \in G$ will transform amongst themselves and will form a (generally reducible) representation. The matrices associated with that representation simply perform permutations of the element of the set S and are obtained from the unit matrix by a permutation of the rows. Moreover, since the point groups are subgroups of $O(n)$, all the elements of S will have the same modulus.
In the one-band case, the Pauli principle forces the singlet pairing functions to be even in $\mathbf{k}$, whereas triplet functions are odd in $\mathbf{k}$. We will focus in what follows on a simple example. A more thorough discussion can be found in Ref. [6].

3.1 C_{4v} symmetry

Let us illustrate the situation of a two-dimensional system on a square lattice with C_{4v} symmetry. The character table is shown on Table 2. Let us consider in succession the representations generated from the vectors $\mathbf{r}=\mathbf{0}$ (on-site), $\mathbf{r}=\hat{\mathbf{x}}$ (first neighbor) and $\mathbf{r}=\hat{\mathbf{x}}+\hat{\mathbf{y}}$ (second neighbor). The representation generated from $\mathbf{r}=\mathbf{0}$ contains a single function, equal to 1, belonging to A_1. The one generated from $\mathbf{r}=\hat{\mathbf{x}}$ contains the four functions

$$\left(e^{ik_x}, e^{ik_y}, e^{-ik_x}, e^{-ik_y}\right) \tag{35}$$

in terms of which the group generators are

$$R(C_4) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix} \quad R(\sigma_x) = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{36}$$

The other elements of the representation are

$$R(C_2) = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad R(\sigma_y) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad R(C_4^{-1}) = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$R(\sigma_d) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad R(\sigma_{d'}) = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \quad R(e) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

From these expression we can compute the projection operators (28). An explicit computation shows that

$$P^{(A_1)} = \frac{1}{4}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix},\ P^{(B_1)} = \frac{1}{4}\begin{pmatrix} 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \end{pmatrix},\ P^{(E)} = \frac{1}{2}\begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix}$$

whereas $P^{(A_2)}$ and $P^{(B_2)}$ vanish. The basis functions we seek are the eigenvectors of these projectors with eigenvalue $+1$

$$A_1 \ :\ (1,1,1,1) \qquad B_1 \ :\ (1,-1,1,-1) \qquad E \ :\ (1,0,-1,0)\ \&\ (0,1,0,-1) \tag{37}$$

which, in terms of the basis (35), are

$$A_1 \ :\ \cos k_x + \cos k_y \qquad B_1 \ :\ \cos k_x - \cos k_y \qquad E \ :\ [\sin k_x, \sin k_y]\,. \tag{38}$$

The representation generated from $\mathbf{r} = \hat{\mathbf{x}} + \hat{\mathbf{y}}$ contains the four functions

$$\left(e^{i(k_x+k_y)}, e^{i(k_x-k_y)}, e^{-i(k_x+k_y)}, e^{-i(k_x-k_y)}\right)\,. \tag{39}$$

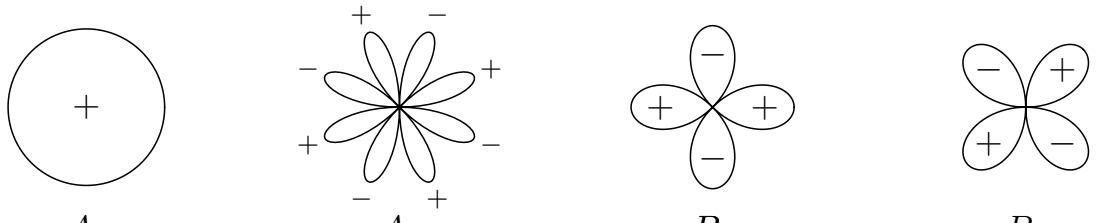
By repeating the same procedure, one finds following basis functions

$$A_1 \ :\ \cos k_x \cos k_y \qquad B_2 \ :\ \sin k_x \sin k_y \qquad E \ :\ [\sin(k_x+k_y), \sin(k_x-k_y)]\,. \tag{40}$$

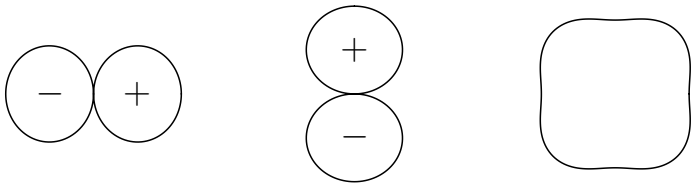
We need to go to the fourth neighbor $\mathbf{r} = 2\hat{\mathbf{x}}+\hat{\mathbf{y}}$ in order to get a basis function belonging to A_2:

$$A_2 \ :\ \sin k_x \ \sin k_y(\cos k_x - \cos k_y) \tag{41}$$

The simplest basis functions for the spatial part of the gap function are shown in the last column of Table 2. Since we are dealing with a single band model, the nodes are solely determined by the structure of the gap function $\Delta(\mathbf{k})$ obtained directly from the functions of Table 2.
The A_1 representation corresponds to isotropic (or s-wave) pairing. The B_1 representation is the well-known d-wave pairing, and the B_2 representation is a variant, rotated by $45°$. The A_2 representation constitutes a more exotic case corresponding to g-wave pairing. Assuming a constant modulus $|\mathbf{k}|$, the gap functions associated to the one-dimensional representations of Table 2 have the following shape as a function of polar angle in the k_x-k_y plane:



The gap functions associated with these representations have respectively 0, 8, 4, and 4 nodes (or zeros) as a function of angle from 0 to 2π. The sign of the function in each lobe is indicated. The E representation is odd under inversion and is therefore associated with triplet superconductivity. The gap function in that case is the doublet $[\sin k_x, \sin k_y]$. Each member of the doublet has two nodal directions. However, it is possible to combine them into complex functions $\sin k_x \pm i \sin k_y$, each behaving like an effective one-dimensional representation of C_{4v}, mapped onto one another by complex conjugation or, physically speaking, time reversal. These complex combinations have no nodes, as the real and imaginary parts do not vanish at the same angle. These gap symmetries are respectively called p_x, p_y and $p_x \pm i p_y$. The corresponding angular dependences are illustrated below, again assuming a constant modulus $|\mathbf{k}|$:



p_x p_y $|p_x \pm i p_y|$

3.2 C_∞ symmetry

In the continuum approximation, i.e., for very long coherence lengths, it is legitimate to assume that a two-dimensional model might have continuous rotation invariance about the z axis. The rotation symmetry, combined with a mirror symmetry across any vertical plane, is effectively the $n \to \infty$ limit of C_{nv}. The irreps of $C_{\infty v}$ are

1. A_1 : the character is 1 for every rotation and reflection.

2. A_2 : the character is 1 for every rotation and -1 for every reflection.

3. E_n ($n \in \mathbb{N}^*$) : the character is $2\cos(n\theta)$ for a rotation of angle θ and 0 for reflections. This is realized by the 2×2 rotation matrices $R(\theta)$ and reflection operators $\Sigma(\theta)$

$$R(\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \qquad \Sigma(\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix} \tag{42}$$

The basis functions corresponding to E_n are the pairs $[\cos n\varphi, \sin n\varphi]$, φ being the polar coordinate on the k_x-k_y plane. These functions have n nodal lines each. The spatially even representations (A_1 and E_{2m}) correspond to singlet superconductivity and the odd representations (A_2 and E_{2m+1}) to triplet superconductivity. The representations $n = 0, 1, 2, \ldots$ are traditionally labeled s, p, d, f, g, etc, like the orbital quantum number in atomic physics. The gap functions in many point groups are labeled likewise, according to the number of nodal lines (e.g., C_{4v} above).

4 Multi-band superconductors

4.1 Band vs orbital basis

Let g denote an element of the point group G. In the absence of SO coupling, its effect on the annihilation operator $c_{\mathbf{r},m,\sigma}$ (Wannier basis) is the following

$$c_{\mathbf{r},m,\sigma} \to c'_{\mathbf{r},m,\sigma} = \sum_{m'} U_{mm'}(g)\, c_{g\mathbf{r},m',\sigma} \tag{43}$$

where $g\mathbf{r}$ is the mapping of site $\mathbf{r}$ under g and $U(g)$ constitutes a N_b-dimensional representation of the group G acting on orbital space. The matrix $U(g)$ is independent of $\mathbf{r}$ by translation invariance, and therefore the same transformation applies in the orbital basis

$$c_{m,\sigma}(\mathbf{k}) \to c'_{m,\sigma}(\mathbf{k}) = \sum_{m'} U_{mm'}(g)\, c_{m',\sigma}(g\mathbf{k})\,. \tag{44}$$

The same symmetry operation is expressed differently in the band basis. From Eq. (6), we find

$$d'_a(\mathbf{k}) = \sum_b \tilde{U}_{ab}(g,\mathbf{k})\, d_b(g\mathbf{k}) \tag{45}$$

where $g\mathbf{k}$ is the image of $\mathbf{k}$ under g and

$$\tilde{U}_{ab}(g,\mathbf{k}) = \sum_{m,m'} V_{a,m}(\mathbf{k})\, V^*_{b,m'}(\mathbf{k})\, U_{mm'}(g)\,. \tag{46}$$

The matrix $\tilde{U}_{ab}(g,\mathbf{k})$ depends on $\mathbf{k}$. Hence the orbital basis makes the group-theoretical analysis much simpler, compared to the band basis, as mentioned above. This is therefore the basis we will use in the following. The physical relevance of the two bases is discussed in Sect. 6.

4.2 The case of Sr_2RuO_4

This formalism for inter-orbital superconductivity can be applied to a model for Sr_2RuO_4 [7–9], summarized in Fig. 3. It is defined on a square lattice, with three Ru t_{2g} orbitals per site. In the figure, these three orbitals (d_{yz}, d_{xz} and d_{xy}) have been drawn on separate planes for clarity. The main hopping terms are illustrated in the figure, but are not so important for our purpose, except for their defining a noninteracting Hamiltonian with D_{4h} symmetry (see Table 3). We use the group D_{4h} even though the model is two-dimensional because (i) we want to cover a three-dimensional extension of the model with weak inter-plane coupling and (ii) the orbitals themselves transform in a nontrivial way under the reflection σ_z across the xy plane. The treatment summarized here is taken from [10].

The group D_{4h} can be generated by successive applications of the elements C_4, σ_x, and σ_z. From Fig. 3 it is obvious that these operations have the following effect on the three orbitals

$$U(C_4) = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad U(\sigma_x) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad U(\sigma_z) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{47}$$

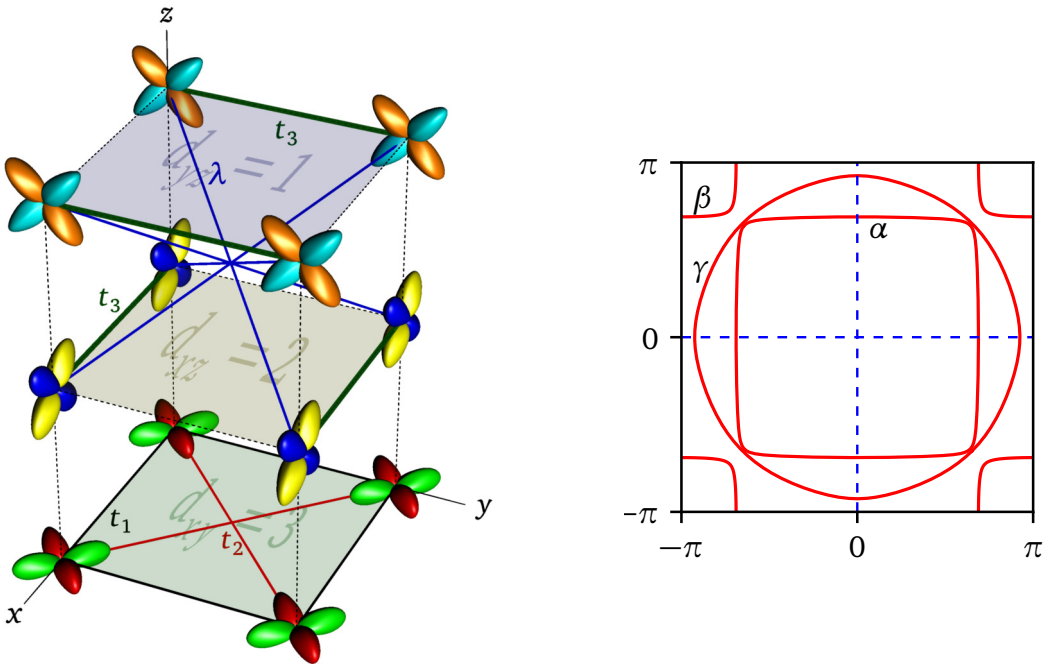


Fig. 3: *Left panel: Schematic view of the SRO unit cell. The three orbitals have been vertically separated for clarity (the model considered is purely two-dimensional). The labels 1,2,3 correspond, respectively, to the d_{yz}, d_{xz}, and d_{xy} orbitals. The different hopping terms ($t_{1,2,3}$ and λ) are illustrated. Right panel: Fermi surface of Sr_2RuO_4 in the simple model illustrated on the left. The α and β bands are a mixture of the d_{xz} and d_{yz} orbitals, whereas the γ band is pure d_{xy}.*

These matrices form, with the rest of the elements of the group, a reducible 3-dimensional representation. From the characters one infers it to be $B_{2g} \oplus E_g$.
The orbital part of the pairing function can be expanded in terms of the following 3×3 matrices

$$\hat{\mathbf{a}}_x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \hat{\mathbf{b}}_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad \hat{\mathbf{c}}_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}$$

$$\hat{\mathbf{a}}_y = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \hat{\mathbf{b}}_y = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \hat{\mathbf{c}}_y = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \tag{48}$$

$$\hat{\mathbf{a}}_z = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \hat{\mathbf{b}}_z = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \hat{\mathbf{c}}_z = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

A general basis state for pairing in orbital space may then be expressed via three vectors $\mathbf{a}$, $\mathbf{b}$,

and $\mathbf{c}$ as

$$O_{mn} = \mathbf{a} \cdot \hat{\mathbf{a}}_{mn} + \mathbf{b} \cdot \hat{\mathbf{b}}_{mn} + \mathbf{c} \cdot \hat{\mathbf{c}}_{mn} \,. \tag{49}$$

The orbital part $O_{mm'}$ transforms as follows under a group operation g

$$O_{mm'} \to \sum_{n,n'} U_{mn}(g)\, U_{m'n'}(g)\, O_{nn'} \quad \text{or} \quad O \to U(g)\, O\, U^T(g) \,. \tag{50}$$

These 9 matrices (48) belong to a 9-dimensional representation of D_{4h}, obtained by taking the tensor products of the matrices (47) with themselves. The content of this representation can easily be shown to be $2A_{1g} \oplus B_{1g} \oplus B_{2g} \oplus E_g$ for symmetric states (spin singlets), and $A_{2g} + E_g$ for antisymmetric states (spin triplets). Again, this classification ignores the spatial part (or rather, supposes that it is invariant).
We can combine these orbital gap functions with spatial functions classified according to Table 3, by taking tensor products and reducing them to irreps using projection operators. Ref. [10] provides tables of singlet and triplet states belonging to each representation, with and without inter-orbital pairing. These tables are too lengthy to reproduce here, but let us consider two examples:

1. Singlet pairing may occur in the constant ($\mathbf{k}$-independent) $\hat{\mathbf{b}}_z$ state, which belongs to the B_{2g} representation of D_{4h}, and is basically pairing between electrons belonging to the d_{xz} and d_{yz} orbitals. This admixture of orbitals occurs in bands α and β of Sr_2RuO_4 (see right panel of Fig. 3), mostly along the diagonals of the Brillouin zone. This pairing would lead to nodes at the intersection of the α and β branches of the Fermi surface with the k_x and k_y axes (dashed lines on the Fig. 3), as the pairing changes sign under C_4 rotations (from Table 3). It therefore has d-wave character.
2. The E_{2u} representation contains many simple triplet gap functions, including $\sin k_z[\hat{\mathbf{b}}_x, \hat{\mathbf{b}}_y]$ and $\hat{\mathbf{a}}_z[\sin k_x, \sin k_y]$. This corresponds to what is usually called $p \pm ip$ superconductivity in this context. The $\hat{\mathbf{a}}_z[\sin k_x, \sin k_y]$ function involves only the γ band and would vanish at two points along the γ band Fermi surface (hence the p-wave epithet). The $\sin k_z[\hat{\mathbf{b}}_x, \hat{\mathbf{b}}_y]$ function vanishes at the equator ($k_z = 0$) and involves admixtures of the d_{xy} and d_{xz} bands ($\hat{\mathbf{b}}_x$) and of the d_{xy} and d_{yz} bands ($\hat{\mathbf{b}}_y$).

4.3 Are nodes imposed by symmetry?

In the one-band case, a symmetry-imposed node occurs in a pairing function that vanishes in some direction because it is odd under certain symmetry operations in the irreducible representation it belongs to. For instance, in the representation B_{1g} of D_{4h} or C_{4v}, the pairing function must be odd under a diagonal reflection σ_d, and must accordingly vanish along the diagonals, which is indeed the case of the standard d-wave function $\cos k_x - \cos k_y$. The pairing function being a scalar, its zeros correspond to nodes. The one-band case is simple because translation invariance allows us to express the order parameter as a scalar function of the wave vector $\mathbf{k}$.
However, strictly speaking, the notion of symmetry-imposed nodes does not make sense in the case of multi-orbital models, with or without spin-orbit coupling.

In a multi-orbital model, the pairing function is a multi-component object: a matrix. That matrix may be odd under a certain symmetry operation, but that does not imply that it must vanish at a fixed point of that operation in momentum space, because the odd character can reside in the orbital part instead of the spatial part. Indeed, the odd character translates into the following transformation property for the pairing function, in the case of, say, the reflection σ_d

$$\Delta_\nu(k_x,k_y,k_z) \to \Delta'_\nu(k_x,k_y,k_z) = \mathcal{U}(\sigma_d)_{\nu\nu'}\,\Delta_{\nu'}(k_y,k_x,k_z) \tag{51}$$

where the index ν labels basis vectors in orbital space (i.e., not the same as the original orbital basis with indices m, m') and $\mathcal{U}$ the orbital part of the representation. In the B_{1g} representation, we therefore have the condition $\Delta'_\nu(k_x,k_y,k_z) = -\Delta_\nu(k_x,k_y,k_z)$, or $[\mathcal{U}(\sigma_d)\boldsymbol{\Delta}(k_y,k_x,k_z)]_\nu = -\Delta_\nu(k_x,k_y,k_z)$, which translates into $[\mathcal{U}(\sigma_d)\boldsymbol{\Delta}(k_x,k_x,k_z)]_\nu = -\Delta_\nu(k_x,k_x,k_z)$ along the diagonal. In the single-orbital case, $\mathcal{U}{=}1$ and that condition implies $\Delta(k_x,k_x,k_z) = 0$. In the multi-orbital case, the orbital part $\boldsymbol{\Delta}$ of the pairing function may be an eigenvector of $\mathcal{U}$ with eigenvalue -1, and this imposes no condition at all on $\Delta_\nu(k_x,k_x,k_z)$. For instance, in our model for Sr_2RuO_4, the pairing function $\hat{\mathbf{a}}_x{-}\hat{\mathbf{a}}_y$, which is wave vector independent, belongs to B_{1g}. The matrix $\mathcal{U}$ in that case exchanges a_x and a_y and is equivalent to -1 in orbital space, which leaves an even (here constant) spatial part.

Another example: the inter-orbital pairing function $\hat{\mathbf{c}}_x \sin k_x + \hat{\mathbf{c}}_y \sin k_y$ belongs to A_{1u} and describes a singlet state that is odd under the reflection σ_z across the xy-plane. Indeed, under this reflection, the orbitals d_{xz} and d_{yz} change sign, and so, according to Eq. (50), do the components $\hat{\mathbf{c}}_x$ and $\hat{\mathbf{c}}_y$, while the functions $\sin k_x$ and $\sin k_y$ are unaffected. The matrix-valued pairing function then takes the form

$$\boldsymbol{\Delta}(k_x,k_y,k_z) = \begin{pmatrix} 0 & 0 & \sin k_y \\ 0 & 0 & \sin k_x \\ -\sin k_y & -\sin k_x & 0 \end{pmatrix} \tag{52}$$

(we ignore spin, which is in a singlet state in this example). The transformation law of that pairing function under σ_z is $\boldsymbol{\Delta} \to \boldsymbol{\Delta}' = U(\sigma_z)\,\boldsymbol{\Delta}\,U^T(\sigma_z)$, where $U(\sigma_z)$ is given in Eq. (47). Therefore $\boldsymbol{\Delta}' = -\boldsymbol{\Delta}$, as it should be in representation A_{1u}. Accordingly, while that pairing function may have nodes, e.g., as a function of k_z, their precise shape or location is not imposed by symmetry.

4.4 The graphene lattice

As a different type of multiband system, let us consider the graphene lattice. It can be seen as a triangular Bravais lattice of elementary hexagons with a basis of two sites (A and B) and lattice basis vectors $\mathbf{e}_1$ and $\mathbf{e}_2$; see Fig. 4.

If the two atoms on sublattices A and B are identical, the point group of the lattice is C_{6v}, when considered from the middle of a hexagonal plaquette. This group has 12 elements in 6 conjugacy classes. All elements may be generated by a $\pi/3$ rotation C_6 and a reflexion σ_v with respect to the horizontal axis of Fig. 4. The character table is shown in Table 4. The particularity

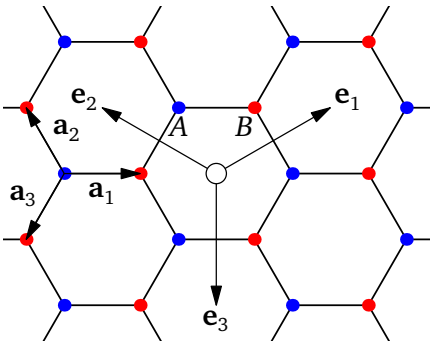


Fig. 4: *The graphene lattice, with two sites (A and B) per unit cell. The lattice basis vectors $\mathbf{e}_{1,2}$ are shown, as well as the elementary bond vectors $\mathbf{a}_i$. The lattice vector $\mathbf{e}_3$ is conveniently defined as $\mathbf{e}_3 = -\mathbf{e}_1 - \mathbf{e}_2$.*

Table 4: *Character table of C_{6v}, with a list of the nearest-neighbor pairing functions for each irrep, expressed as function of $k_i = \mathbf{k}\cdot\mathbf{e}_i$. Irreps A_2 and B_2 need longer-range pairing to appear.*

	e	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$	basis functions
A_1	1	1	1	1	1	1	$1\ ,\ \cos k_1 + \cos k_2 + \cos k_3$
A_2	1	1	1	1	−1	−1	
B_1	1	−1	1	−1	1	−1	$\sin k_1 + \sin k_2 + \sin k_3$
B_2	1	−1	1	−1	−1	1	
E_1	2	1	−1	−2	0	0	$[\sin k_1 - \sin k_2\ ,\ \sin k_1 - \sin k_3]$
E_2	2	−1	−1	2	0	0	$[\cos k_1 - \cos k_2\ ,\ \cos k_1 - \cos k_3]$

of this system is that the group transformations do not leave the unit cell intact (a unit cell may be defined as a pair of neighboring A and B sites, and the ambiguity in defining these pairs breaks the C_{6v} symmetry). This makes the separation (13) into orbital and momentum variables awkward. In this case it is therefore preferable to work directly in real space and to incorporate orbital and Wannier indices into a single spatial index $\mathbf{r}$, belonging to the A or B sublattices (the sites $\mathbf{r}$ therefore do not form a Bravais lattice). If we ignore the spin part, the pairing amplitude is then simply a function $\Delta_{\mathbf{r},\mathbf{r}'}$. Translation invariance imposes the condition $\Delta_{\mathbf{r}+\mathbf{e}_i,\mathbf{r}'+\mathbf{e}_i} = \Delta_{\mathbf{r},\mathbf{r}'}$. We will define $\mathbf{b} = \mathbf{r}' - \mathbf{r}$ as the bond vector, and it turns out that this vector uniquely characterizes the pairing amplitude, even though the set of $\mathbf{b}$ vectors does not form a Bravais lattice. We can therefore express the pairing function as $\Delta_{\mathbf{b}}$ and the action of a group element $g \in G$ on such a function may be represented as

$$\Delta_{\mathbf{b}} \longrightarrow \sum_{\mathbf{b}'} R_{\mathbf{b},\mathbf{b}'}(g)\Delta_{\mathbf{b}'} \tag{53}$$

Because the point group preserves the norm of $\mathbf{b}$, we can restrict our analysis to sets of bond vectors of the same length.

The simplest possibility beyond the trivial one-site pairing $\mathbf{b} = 0$ is nearest-neighbor pairing, with $\mathbf{b} = \pm\mathbf{a}_i$ ($i = 1, 2, 3$) where the elementary bond vectors $\mathbf{a}_i$ are defined on Fig. 4. It is also

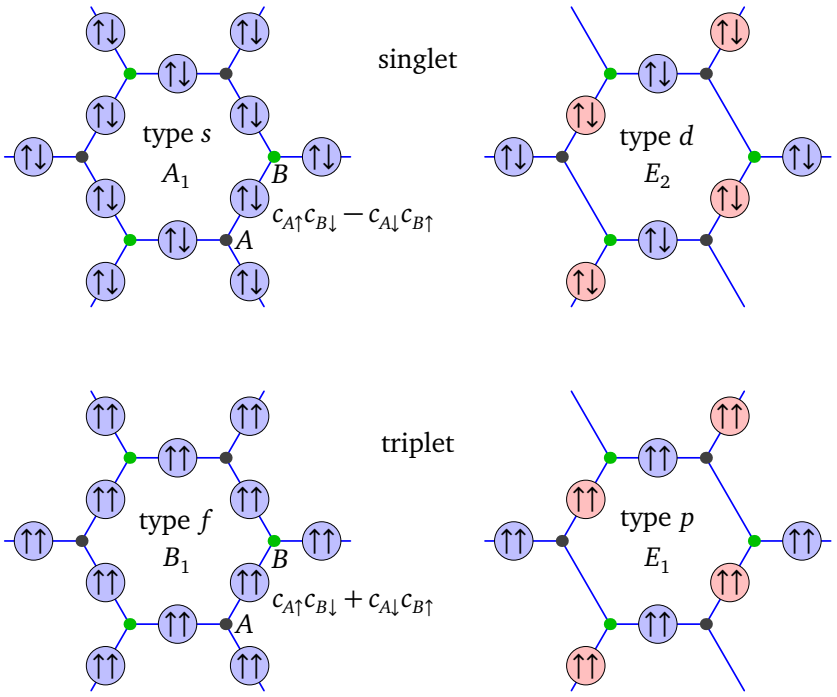


Fig. 5: *The simplest pairing functions on the graphene lattice. Each pairing (singlet or triplet) lives on nearest-neighbor bonds. The color (blue = +, red = −) represents the sign of the pairing amplitude. Note that rotating by $\pi/3$ exchanges the A and B sublattices, and therefore changes the sign of the triplet amplitude $c_{A\uparrow}c_{B\downarrow} + c_{A\downarrow}c_{B\uparrow}$, which justifies, in particular, the f-wave label.*

the predominant pairing to expect in a strongly correlated model with a large on-site repulsion U. These six bonds are associated with a multiplet of six pairing functions $\Delta_{\mathbf{b}} = \delta_{\mathbf{b},\pm\mathbf{a}_i}$ (i=1, . . . , 3). The explicit representation matrices $R(g)$ are simple to construct, and so are the projection operators $P^{(\mu)}$ associated with the 6 irreps of C_{6v}.

The mathematics are the same as for a one-band model defined on a triangular lattice. In that case, the pairing functions are written, in the usual language, in the last column of Table 4, as a function of the wavevector components $k_i = \mathbf{k} \cdot \mathbf{e}_i$. There is a simple correspondence between these functions and the graphene pairing functions $\Delta_{\mathbf{b}}$:

$$e^{\pm ik_j} \longleftrightarrow \delta_{\mathbf{b},\pm\mathbf{a}_j} \tag{54}$$

For instance, the nearest-neighbor graphene pairing function belonging to the B_1 representation would be

$$\Delta_{\mathbf{b}}(B_1) = \delta_{\mathbf{b},\mathbf{a}_1} - \delta_{\mathbf{b},-\mathbf{a}_1} + \delta_{\mathbf{b},\mathbf{a}_2} - \delta_{\mathbf{b},-\mathbf{a}_2} + \delta_{\mathbf{b},\mathbf{a}_3} - \delta_{\mathbf{b},-\mathbf{a}_3} \ . \tag{55}$$

The functions associated with A_1 and E_2 are even under a spatial inversion (here equivalent to the π-rotation C_2), and are therefore appropriate for singlet pairing, whereas those associated with B_1 and E_1 are odd and are appropriate for triplet pairing. These possibilities are illustrated schematically in Fig. 5, taken from Ref. [11]. Based on the number of times the bond amplitude changes sign as a function of angle, representations A_1, B_1, E_1, and E_2 can be labeled as s, f, p, and d-wave, respectively.

5 Superconductors with spin-orbit interaction

5.1 One-band model with Rashba coupling

Let us consider a simple one-band model on a square lattice with a Rashba SO coupling

$$H_0 = \sum_{\mathbf{k}} C^\dagger_{\mathbf{k}} \Big(\varepsilon(\mathbf{k}) + \kappa\big(\tau_y \sin k_x - \tau_x \sin k_y\big) \Big) C_{\mathbf{k}} \tag{56}$$

where $C_{\mathbf{k}} = (c_{\mathbf{k}\uparrow}, c_{\mathbf{k}\downarrow})$. Assuming nearest-neighbor hopping t, the dispersion relation is $\varepsilon(\mathbf{k}) = -2t(\cos k_x + \cos k_y)$. This model has C_{4v} symmetry and, without the SO interaction, the gap functions are classified in accordance with Sect. 3.1. Because of the κ term, under a point group transformation g, both the orbital and spin indices are affected

$$c_{\mathbf{r},\sigma} \to c'_{\mathbf{r},\sigma} = \sum_{\sigma'} S_{\sigma\sigma'}(g)\, c_{g\mathbf{r},\sigma'} \tag{57}$$

where $g\mathbf{r}$ is the image of $\mathbf{r}$ by g. Under the $\pi/2$ rotation C_4, we can apply the usual expression for $SU(2)$ spin rotations and

$$S(C_4) = \cos\frac{\pi}{4} + i\sigma_z \sin\frac{\pi}{4} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1+i & 0 \\ 0 & 1-i \end{pmatrix} \tag{58}$$

As for the reflection σ_x, it maps (k_x, k_y) into $(-k_x, k_y)$ and therefore should have the following effect

$$S^\dagger\, \tau_x\, S = \tau_x \qquad S^\dagger\, \tau_y\, S = -\tau_y\ . \tag{59}$$

A solution is to set $S(\sigma_x) = i\tau_x$.

The matrices $S(g)$ generated from $S(C_4)$ and $S(\sigma_x)$ from a *spin representation* of C_{4v}. Such representations are not listed in the character table 2. In particular, within such a spin representation, the fourth power $S(C_4)^4$ is -1, not 1.[6] The tensor product of this spin representation with itself yields symmetric and antisymmetric unitary representations, characterized by the $\mathbf{d}$-vector basis (15), namely:

1. A_1, with gap function $\hat{\mathbf{d}}_0$ (singlet)
2. A_2, with gap function $\hat{\mathbf{d}}_z$ (triplet).
3. E, with gap function $[\hat{\mathbf{d}}_x, \hat{\mathbf{d}}_y]$ (triplet).

(the projection operator technique illustrated in Sect. 3.1 can be applied equally well to this situation.) The first (A_1) is antisymmetric under exchange of the quantum numbers of the two electrons, the other two (A_2 and E) are symmetric. These unitary representations can in turn be tensored with orbital and spatial representations, provided the overall pairing function is antisymmetric. Table 5 lists the simplest gap functions coming from this exercise. In particular, the usual singlet d-wave function belonging to B_1 would generically have a small triplet admixture with the function $\hat{\mathbf{d}}_x \sin k_y + \hat{\mathbf{d}}_y \sin k_x$. Would this affect the nodes? In general yes, if the strength of the Rashba SO coupling κ is large enough.

[6] This is the analog for point groups of the properties of spin rotations in the continuum. In some sense, such spin representations are the "square roots" of the usual representations: their tensor products with themselves are unitary representations. They are *projective* (or *ray*) representations.

Table 5: *On-site and first-neighbor gap functions for a square lattice with C_{4v} symmetry and spin-orbit coupling.*

Irrep	Basis functions
A_1	$\hat{\mathbf{d}}_0 \quad , \ (\hat{\mathbf{d}}_x \sin k_y - \hat{\mathbf{d}}_y \sin k_x)$
A_2	$\hat{\mathbf{d}}_x \sin k_x + \hat{\mathbf{d}}_y \sin k_y$
B_1	$\hat{\mathbf{d}}_0(\cos k_x - \cos k_y) \ , \ \hat{\mathbf{d}}_x \sin k_y + \hat{\mathbf{d}}_y \sin k_x$
B_2	$\hat{\mathbf{d}}_x \sin k_x - \hat{\mathbf{d}}_y \sin k_y$
E_1	$\hat{\mathbf{d}}_z[\sin k_x, \ \sin k_y]$

5.2 Sr_2RuO_4

The case of Sr_2RuO_4 provides us with a more complex application of the above ideas. The spin-orbit term appropriate for Sr_2RuO_4 is

$$H_{\rm SO} = i\,\frac{\kappa}{2} \sum_{\mathbf{r}} \sum_{l,m,n} \varepsilon_{lmn}\; c^\dagger_{\mathbf{r},l,\sigma}\, c_{\mathbf{r},m,\sigma'}\, \tau_{n,\sigma\sigma'} \tag{60}$$

where τ_n is the $n^{\rm th}$ Pauli matrix, acting on spin indices. Under a general D_{4h} transformation, the spin-orbit term becomes

$$i\frac{\kappa}{2} \sum_{\mathbf{r}} \sum_{l,m,n} \varepsilon_{l'm'n}\, U^*_{l'l}\, U_{m'm}\; c^\dagger_{\mathbf{r},l,\sigma}\, c_{\mathbf{r},m,\sigma'}\; S^*_{\alpha\sigma}\, S_{\alpha'\sigma'}\, \tau_{n,\alpha\alpha'} \ . \tag{61}$$

In order for the spin-orbit term to be invariant, the spin rotation matrix S must belong to a spin representation of the group such that

$$\begin{aligned} S^\dagger\, \tau_n\, S &= R_{nn'}\, \tau_{n'} \\ \varepsilon_{l'm'n}\, U^*_{l'l}\, U_{m'm} &= R^{-1}_{nn'}\, \varepsilon_{lmn'} \end{aligned} \tag{62}$$

It can be shown that, for the generators of D_{4h},

$$S(C_4) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1{+}i & 0 \\ 0 & 1{-}i \end{pmatrix} \qquad S(\sigma_x) = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \qquad S(\sigma_z) = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \tag{63}$$

We then proceed like in the previous section: we build tensor product representations for pairs of electrons, and tensor those with irreps for the spatial part of the gap function. The resulting gap functions are numerous. Singlet and triplet gap functions can coexist in the same irrep, and new ones arise. For instance, in the B_{1g} (a.k.a. d-wave) representation, we find the singlet gap function $\hat{\mathbf{a}}_z \hat{\mathbf{d}}_0(\cos k_x - \cos k_y)$ and the triplet gap function $\hat{\mathbf{c}}_z \hat{\mathbf{d}}_z(\cos k_x - \cos k_y)$. Since spin is not conserved separately, not only do singlet and triplet components coexist in the same irrep, but different directions of the $\mathbf{d}$-vector can also coexist. For instance, the function $\hat{\mathbf{c}}_x \hat{\mathbf{d}}_x + \hat{\mathbf{c}}_y \hat{\mathbf{d}}_y$ also belongs to the same representation. Details can be found in [10].

6 Final remarks

Group theory is a powerful tool for classifying superconducting pairing states, especially in the presence of many orbitals. However, it must be kept in mind that it makes no *dynamical* predictions. It does not inform us on which of the gap functions is preferred on the basis of a particular model; other tools are necessary. We can, however, venture in the following general considerations in the presence of many bands: For weakly correlated materials, the band description is more natural than the Wannier (orbital) description. We would then expect pairing to occur at weak energies, i.e., for wave vectors close to the Fermi surface. Since pairing occurs between opposite wave vectors, this nearly restricts it to occur within each band separately (assuming time reversal symmetry, i.e., that $-\mathbf{k}$ belongs to the Fermi surface if $\mathbf{k}$ does). What appears as inter-orbital pairing might then be merely intra-band pairing.
On the other hand, for strongly correlated materials, pairing may occur on a wider energy scale, in which case the relation to Fermi surfaces is less important and the Wannier description is more appropriate. In that case, we also expect pairing to have a shorter range and the short-range pairing functions found in the general method exposed here are more relevant. The case of Sr_2RuO_4 is particularly interesting: that material is undoubtedly strongly correlated. At the same time, its three bands (α, β, γ) have Fermi surfaces that almost touch along the diagonals (Fig. 3). In an intermediate-coupling situation, inter-orbital pairing would therefore be expected to occur in the vicinity of these diagonal areas where the three Fermi surfaces almost meet.

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