Singlet and triplet pairing states

It is convenient to separate the four spin components of the pairing field into a scalar $\Delta_{\mathbf{k}}$ and a vector $\mathbf{d}_{\mathbf{k}}$ as follows

$$\Delta_{\sigma\sigma'}(\mathbf{k}) = (\Delta_{\mathbf{k}} I + \sigma.\mathbf{d}_{\mathbf{k}})\mathbf{i}\sigma_{\mathbf{y}}$$

where $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ is a vector of Pauli matrices and I is the 2x2 unit matrix.
Explicitly for singlet pairing

$$\begin{pmatrix} \Delta_{\uparrow\uparrow}(\mathbf{k}) & \Delta_{\uparrow\downarrow}(\mathbf{k}) \\ \Delta_{\downarrow\uparrow}(\mathbf{k}) & \Delta_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix} = \begin{pmatrix} 0 & \Delta_{\mathbf{k}} \\ -\Delta_{\mathbf{k}} & 0 \end{pmatrix}$$

where $\Delta_{\mathbf{k}} = \Delta_{-\mathbf{k}}$

Singlet and triplet pairing states (2)

And for triplet pairing

$$\begin{pmatrix} \Delta_{\uparrow\uparrow}(\mathbf{k}) & \Delta_{\uparrow\downarrow}(\mathbf{k}) \\ \Delta_{\downarrow\uparrow}(\mathbf{k}) & \Delta_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix} = \begin{pmatrix} -d_x + id_y & d_z \\ d_z & d_x + id_y \end{pmatrix}$$

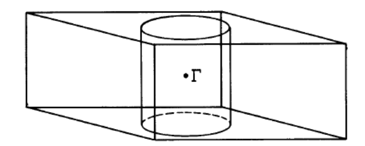
where $\mathbf{d}_{\mathbf{k}} = -\mathbf{d}_{-\mathbf{k}}$
The fact that these are scalar and vectors under rotation (in spin-space) follows from the mappring of the $SU(2)$ group of spin $1/2$ particles to the $SO(3)$ rotation group in 3 dimensions.

Crystal point group symmetries

A similar argument can be made for the **k** dependenes of the pairing within the crystal's Brillouin zone. Here the relevant classification is by *irreducible representations* of the crystal point group. The theory of representations is a whole course in itself, but the basic ideas are relatively straightforward.

The crystal will have a set of rotation axes (C_2, C_3, C_4 or C_6) and mirror planes (σ_v). Together these form a group.

These operations transform functions in the Brillouin zone $f(\mathbf{k})$ in different ways. Functions can be classified into components which are distinct by symmetry (eg even/odd).



Crystal point group symmetries (2)

The *character table* of the group lists the irreducible representations, and usually also the simplest functions which transform according to the symmetries. Eg for D_4 (tetragonal crystals)

	E	C_2	$2C_4$	$2C_2'$	$2C_2''$	
A_1	1	1	1	1	1	const.
A_2	1	1	1	-1	-1	$xy(x^2-y^2)$
B_1	1	1	-1	1	-1	xy
B_2	1	1	-1	-1	1	x^2-y^2
E	2	-2	0	0	0	$\{x,y\}$

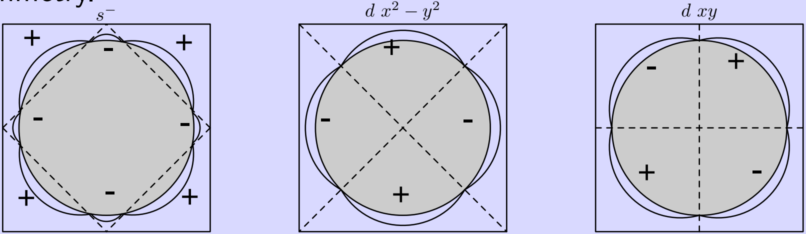
Character=Tr of matrix for given irrep

Crystal point group symmetries (3)

The gap function $\Delta_\mathbf{k}$ of the superconductor will transform as one of the irreducible representations of the point group, eg

$$\Delta_\mathbf{k} = \Delta f(\mathbf{k})$$

where $f(\mathbf{k})$ is a basis function for the relevant symmetry.
In many (not all) cases gap nodal points are required by symmetry.



A Ginzburg Landau approach

Let us now reformulate these symmetry arguments in terms of the Ginzburg Landau theory of superconductivity.

- This is valid near to T_c
- Assuming non accidental degneracy of order parameters we can determine the gap function at T_c and also below it.
- Agin this is general and does not assume any specific pairing model or a mean field (eg BCS) approximation.

A Ginzburg Landau approach (2)

The original Ginzburg Landau theory assumed a single complex order parameter, here η. The free energy in the superconducting state is

$$f_s - f_n = \frac{\hbar^2}{2m}|\nabla\eta|^2 + \alpha(T)|\eta|^2 + \frac{\beta}{2}|\eta|^4$$

where $\eta(\mathbf{r})$ is assumed to vary slowly on microscopic length scales ($\xi_0 >> a$). T_c is the temperature where $\alpha(T)$ becomes negative.

A magnetic vector potential can be included by the usual replacement

$$-i\hbar\nabla \to -i\hbar\nabla - 2e\mathbf{A}$$

signifying a charge $2e$ condensate.

A Ginzburg Landau approach (3)

This is true for s-wave superconductivity, and also for any system with a pairing in a *one-dimensional* irreducible representation of the symmetry group. For example $d_{x^2-y^2}$ pairing in the cuprates.

For a two, three or higher dimensional irreducible representation then we have a set of order parameters η_i, $i = 1, 2 \ldots$.

We must generalize the Ginzburg Landau theory to this case.

Again group theory helps us find the relevant terms.

A Ginzburg Landau approach (4)

Consider first the quadratic term. If there are multiple order parameters η_i then it might have the form

$$f_s - f_n = \sum_{ij} \alpha_{ij}(T)\eta_i^* \eta_j$$

where α_{ij} is a temperature dependent matrix.
But by the central defining principle of irreducible representations, any matrix can be decomposed by unitary transformations into a block diagonal form

$$\alpha_{ij} = \begin{pmatrix} \alpha^{\Gamma} & 0 & 0 \\ 0 & \alpha^{\Gamma'} & 0 \\ 0 & 0 & \dots \end{pmatrix}$$

where Γ, Γ' etc. are irreducible representations of the symmetry group.

A Ginzburg Landau approach (5)

The different irreducible representations will have distinct transition temperatures T_c, and again the one with the highest temperature determines the pairing symmetry.
Within a single irrep. Γ the matrix α^Γ is is just a constant times the identity matrix. Therefore the quadratic term must have the form

$$f_s - f_n = \alpha^\Gamma(T) \sum_i \eta_i^* \eta_i$$

where $\alpha^\Gamma(T)$ is positive for $T > T_c$ and negative for $T < T_c$.
If a second irreducible representation also becomes superconducting, this must (almost) always occur at a second phase transition $T_{c2} < T_c$. The heavy fermion system UPt_3 might be an example of this (Garg).

A Ginzburg Landau approach (6)

The nature of the state immediately below T_c is determined by the *quartic* terms in the Ginzburg Landau theory.
The form of these is again determined by goup theory, they are *quartic invariants* of the symmetry group.

$$f_s - f_n = \alpha^{\Gamma}(T) \sum_i \eta_i^* \eta_i + \frac{1}{2} \sum_{ijkl} \beta_{ijkl} \eta_i^* \eta_j^* \eta_k \eta_l$$

For example from the E representation of D_{4h}, we have to consider the product reresentation, and discover how many terms in the product are invariants of the full symmetry group:

$$E \times E \times E \times E = 4A_1 + \ldots$$

A Ginzburg Landau approach (7)

In this case one of the invariants is identically zero, and so there are three quartic terms. The minimum free energy is dependent on these parameters.

Three types of minima can occur

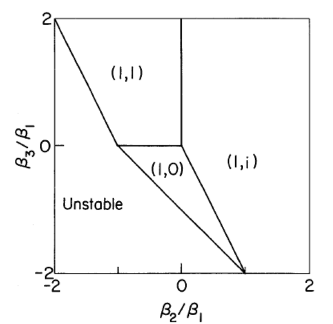
$\Delta_{\mathbf{k}} \sim k_x k_z$

$\Delta_{\mathbf{k}} \sim (k_x + k_y)k_z$

$\Delta_{\mathbf{k}} \sim (k_x + ik_y)k_z$

or for odd parity etc.

$\mathbf{d}_{\mathbf{k}} \sim k_x + ik_y$



Δ.

A Ginzburg Landau approach (8)

The form of the gradient terms is also determined by group theory:

$$
\begin{aligned}
f_s - f_n &= \sum_{ijkl} \frac{\hbar^2}{2m_{ijkl}} \nabla_i \eta_j^* \nabla_i \eta_j \\
&\quad + \alpha^\Gamma(T) \sum_i \eta_i^* \eta_i + \frac{1}{2} \sum_{ijkl} \beta_{ijkl} \eta_i^* \eta_j^* \eta_k \eta_l
\end{aligned}
$$

Now we also have to determine how ∇ decomposes into the irreducible representations of the group, eg in D_{4h}

$$(\nabla_x, \nabla_y) \sim E$$

$$\nabla_z \sim A_2$$