

PHASE TRANSITIONS FOR UNCONVENTIONAL SUPERCONDUCTIVITY

¹A. Ekpeko, ²S.E. Iyayi & ³E. Aiyohuyim

¹Department of Physics, Delta state University, Abraka.

²Department of Physics, Ambrose Alli, University Ekpoma.

³Department of Physics, University of Benin.

ABSTRACT

The transition temperature of the gap functions of two irreducible representations are very close to each other, but it is not possible to consider them independently. We have to extend the Ginsburg-landau free energy to both representations, including also coupling terms between the order parameters

1. INTRODUCTION

The transition temperatures of the gap functions of two irreducible representations are very close to each other, it is not possible to consider them independently. We have to extend the Ginsburg-Landau free energy to both representation, including also coupling terms between the order parameters, where β_1, β_1^1 and θ_i are real coefficients that are material dependent. The coefficients of the second-order terms are

$$A_i(T) = a^i \left(\frac{T}{T_i} - 1 \right) [T_i - T_c(\Gamma_i)]$$

A general analysis of the phase transitions for all possible values of the coefficients is rather complicated in this system and even numerically hard to handle, since a large number of local minima of f make the search for the global minimum rather difficult. Therefore, we restrict ourselves to some typical cases which allow simple analytic argumentation. The superconducting states of Γ_5 representation are determined by the relation between β_2 and β_3 .

The different types of state are separated by lines in the $\beta_2^i - \beta_3^i$ plane. However, if we include coupling terms to other representation, these lines are in general modified and the regions close to them are not at all simple to analyse. To avoid such complications

$$F(\eta) = F_r(\eta(\Gamma, m)) + F_{r,i}(\eta(\Gamma', m)) + F_{\Gamma,\Gamma'}(\eta(\Gamma, m), \eta(\Gamma', m)) \quad (1)$$

The coupling terms $F_{\Gamma,\Gamma'}$ can be derived again by applying the conditions that F is invariant under all symmetry transformations. The procedure is analogous to earlier cases. No second-order coupling terms exist, since the decomposition of $\Gamma \otimes \Gamma'$ never leads to scalar terms Γ_i components. The next higher order is four, where we have to decompose four products

$$\begin{aligned} &\Gamma^* \otimes \Gamma \otimes \Gamma^* \otimes \Gamma^i \\ &\Gamma^* \otimes \Gamma^* \otimes \Gamma' \otimes \Gamma' + \text{c.c.}, \\ &\Gamma^* \otimes \Gamma' \otimes \Gamma^* \otimes \Gamma' + \text{c.c.}, \\ &\Gamma^* \otimes \Gamma \otimes \Gamma^* \otimes \Gamma' + \text{c.c.} \end{aligned}$$

The asterisks again denote the complex conjugate order parameter basis. Note that in these combinations the invariance under time reversal and $U(1)$, gauge transformation is satisfied. A complete list of all terms of all combinations of representations in the cubic point group can be found in Sigrist and Rice (1989) and for other point groups in Sahu, Lagner, and George (1988).

2. THEORETICAL CONSIDERATIONS AND CALCULATIONS

It is convenient for further analysis to write the complete free energy in the parameterization $\eta(\Gamma_i) = |\eta| e^{i\phi}$ and $\eta(\Gamma_5, m) = |\eta_m| e^{i\phi m}$, so that we obtain the free energy density.

$$\begin{aligned}
f = & A_i(T)|\eta|^2 + \beta|\eta|^4 + A_5(T)(|\eta_1|^2 + |\eta_2|^2 + |\eta_3|^2 + |\eta_3|^2) \\
& + \beta_1(|\eta_1|^2 + |\eta_2|^2 + |\eta_3|^2) \\
& + \beta_2(|\eta_1|^4 + |\eta_2|^4 + |\eta_3|^4 + 2|\eta_1|^2|\eta_2|^2 \cos(2\phi_1 + 2\phi_2) \\
& + 2|\eta_2|^2|\eta_3|^2 \cos(2\phi_2 + 2\phi_3) + 2|\eta_3|^2|\eta_1|^2 \cos(2\phi_3 + 2\phi_1)) \\
& + \beta_3(|\eta_1|^2|\eta_2|^2|\eta_3|^2 + |\eta_3|^2|\eta_1|^2) + \theta_1|\eta_1|^2(|\eta_1|^2 + |\eta_3|^2) \\
& + \theta_2|\eta_1|^2[(|\eta_1|^2 \cos(2\phi_1 + 2\phi) + (|\eta_2|^2 \cos(2\phi_2 + 2\phi) \\
& + (|\eta_3|^2 \cos(2\phi_3 + 2\phi))] \\
& + \theta_2|\eta_1||\eta_2||\eta_3|[\cos(\phi_3 - \phi_2)\cos(\phi_1 - \phi) + (\phi_2 - \phi)\cos(\phi_3 - \phi) \\
& + (\phi_3 - \phi)\cos(\phi_2 - \phi)]
\end{aligned} \tag{3}$$

We concentrate below on regions far from any original borderline in the $\beta'_2 - \beta'_3$ diagram. As a first example, let us consider the case $0 \ll \beta'_3$ and $4\beta'_1 < 4\beta'_2 \ll 4\beta'_3$. With the assumptions $T_5 > T_1$, the stable superconducting state immediately below the onset of superconducting at T_5 is clearly a single representation (*SR*) state,

$$|\eta_1|^2 = \frac{A_5(T)}{2(\beta_1 - \beta_2)} \text{ and } \eta = \eta_2 = \eta_3 = 0, \tag{4}$$

which is threefold degenerate with the symmetry $D_{4h}(\Gamma_4)$. This state is generally not stable for all lower temperatures. For example, an additional second order (continuous) transition can occur at certain lower temperature, say T_1 , leading to a combined representation (CR) state where the Γ_1 order parameter also becomes finite,

$$\begin{aligned}
|\eta_1| &= \frac{A_1 Q - 2\beta_1 A_5}{4\beta_1(\beta'_1 + \beta'_2) - Q}, \quad \eta_2 = \eta_3 = 0 \\
|\eta| &= \frac{A_5 Q - 2(\beta'_1 + \beta'_2)A_1}{4\beta_1(\beta'_1 + \beta'_2) - Q^2}, \\
\phi_1 - \phi &= \begin{cases} 0, \pi, \theta_2 < \theta_1 \\ \frac{x}{2}, \frac{3\pi}{2}, \theta_2 > \theta_1 \end{cases}
\end{aligned} \tag{5}$$

with $Q = \theta_1 - |\theta_2|$. The transition point T_1 is determined as the temperature where $|\eta|^2$ vanishes in these equations. This corresponds to the zero of the effective second-order term of η obtained in f by inserting $|\eta_1|$ from equation (4)

$$T_1' = T_1 \frac{1-G}{1-GT_1/T_5} \tag{6}$$

$$\text{with } G = \frac{Q}{2(\beta_1 + \beta_2)} \Gamma_5 \rightarrow \Gamma_1 \otimes \Gamma_5$$

The transition is defined for $Q < 2(\beta'_1 + \beta'_2)$, and T_1' is enhanced compared with T_1 if Q is “attractive” and suppressed if Q is repulsive (>0). Obviously, at this transition the point group symmetry is broken, and for $\theta_2 > 0$ even time-reversal symmetry is lost

$$C_{2h}(\Gamma_1) \text{ for } \theta_2 < 0 \text{ and } D_{4h}(\Gamma_1 \otimes \Gamma_4) \text{ for } \theta_2 > 0, \text{ both sixfold degenerate}]$$

A further transition is possible to the *SR* state of Γ_1 ,

$$|\eta|^2 = \frac{A_4(T)}{2\beta_4}, \quad \eta_1 = \eta_2 = \eta_3 = 0 \tag{7}$$

with the transition point

$$T_5'' = T_5 \frac{1-G''}{1-G''/T_1} \tag{8}$$

with $G'' = \frac{Q}{2\beta_1}$ $\Gamma_1 \rightarrow \Gamma_1 \otimes \Gamma_5$

determined by the zero of the numerator of $|\eta|^2$ in equation (5). The transition can take place only under the assumption $Q > 2\beta_1 > 0$. In that case the coupling between the two superconducting order parameters is repulsive, and because of $\beta_1 < \beta'_1 + \beta'_2$ the Γ_1 order parameter is able to suppress the Γ_5 order parameter. The CR state has the existence condition $T''_1 > T''_5$ which can also be expressed as $Q^2 < 4\beta_1(\beta'_1 + \beta'_2)$. If all these conditions are fulfilled, we find three consecutive second-order transition normal state $\rightarrow SR(\Gamma_5) \rightarrow CR(\Gamma_1 \otimes \Gamma_5) \rightarrow SR(\Gamma_1)$.

In the case $T'_5 > T'_1$, for which the CR state cannot exist a direct transition can take place between the $SR(\Gamma_5)$ and the $SR(\Gamma_1)$ states. Generally this transition is discontinuous, a first-order transition. The transition temperature T is defined as the point where the free energies of both SR are equal.

$$F_{\Gamma_1}(\bar{T}) = \frac{-A_1^2(\bar{T})}{4\beta_1} = F_{\Gamma_5}(\bar{T}) = \frac{-A_5^2(\bar{T})}{4(\beta'_1 + \beta'_2)} \tag{9}$$

For a physical solution ($T_5 > \bar{T} > 0$) the condition $\beta'_1 > \beta'_1 > \beta_1$ is required. Then it leads to a transition series normal state $\rightarrow SR(\Gamma_5) \rightarrow SR(\Gamma_1)$.

In fig 1(a)-1(d), the qualitative phase diagram of the transition is drawn for varying Q {figs 1(a) and 1(b) and varying $2(\beta'_1 + \beta'_2)$ fig (c) and 1(d)}. Regions where $SR\Gamma_5$ state is stable for all temperature below T_5 can also be found in this phase diagram. Note that an examination of the opposite case $T_1 > T_5$ leads to completely analogous conclusion

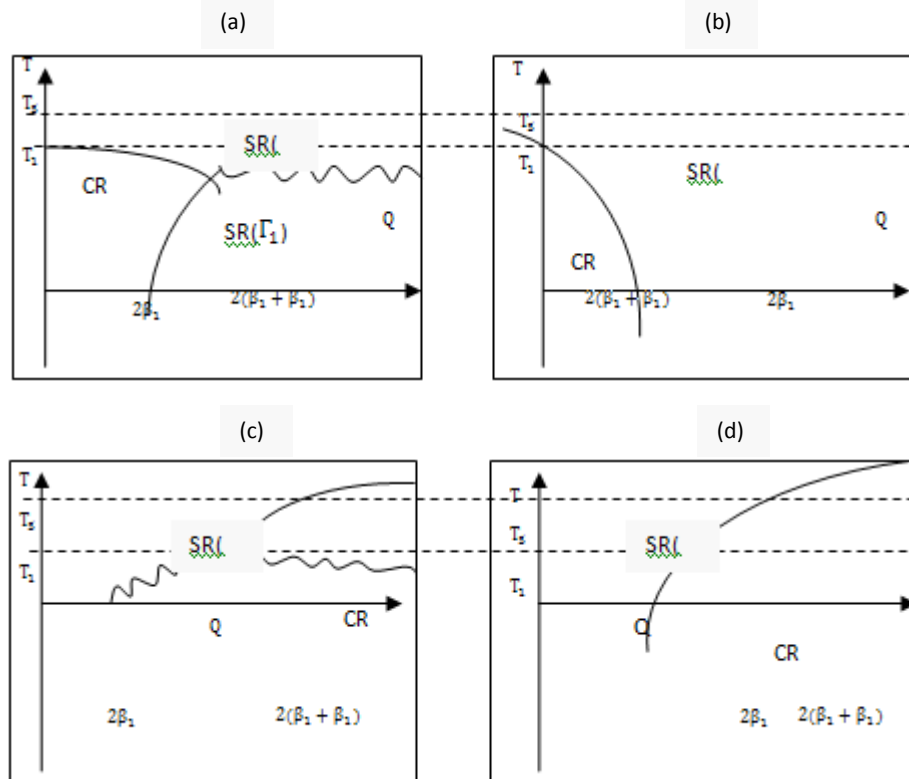


Figure 1(a-d). Phase diagrams of additional phase transitions in the Ginzburg Landau theory combining the two representation Γ_1 and Γ_5 : T versus the coupling constant Q for (a) $\beta_2 < \beta'_1 + \beta'_2$ and (b) $\beta_2 > \beta'_1 + \beta'_2$; T versus the parameter $2(\beta'_1)_1 + \beta'_2$ for (c) $2\beta_1 < Q$ and (d) $2\beta_1 > Q$.

In this example, the conditions $0 \ll \beta_3$ and $4\beta'_1 < 4\beta'_2 \ll \beta'_3$ have been chosen so that only coupling terms are involved which contain the two order parameters in the same order. The term with the coefficient θ_3 which is linear in the Γ_1 order parameter and in the third-order Γ_5 order parameter, gives no contribution, since it requires that all three components of the Γ_5 order parameter be finite, which is energetically rather unfavourable in this parameter range. To see the mode of operation of this type of coupling terms (unequal, order coupling), we consider the case $0 > \beta'_2, \beta'_3$ [also far from the borderlines in the β, β'_3 phase diagram, but additionally $\beta'_1 > -\left(\beta'_2 + \beta'_3/3\right)$],

which leads to a state with $\eta_1 = \eta_2 = \eta_3 = \eta$ by minimization of $F_{\Gamma_5}[D_{3d}(\Gamma_1)]$. Making use of this form of the Γ_5 order parameter, we can write the free-energy density f equation (3) as

$$f(\eta, \bar{\eta}) = A_1(T)|\eta|^2 + \beta_1|\eta|^4 + 3[A_5(T)|\eta|^2 + [3(\beta'_1 + \beta'_2) + \beta'_3]|\eta|^4] + [\theta_1 + \theta_2 \cos(2\bar{\phi} - 2\phi)]|\eta|^2|\eta|^2 + 3\theta_3 \cos(\bar{\phi} - \phi)|\eta||\eta|^2 \quad (10)$$

where we set $\phi_1 = \phi_2 = \phi_3 = \phi$. We assume for our discussion that the form of this Γ_5 order parameter is not changed for any temperature. For $T_5 > T_1$ we would expect that, in analogy with the former example immediately below T_5 the $SR(\Gamma_5)$ state would appear with

$$|\eta|^2 = \frac{-A_5(T)}{6(\beta'_1 + \beta'_2) + 2\beta'_3} \quad (11)$$

However, this is prohibited by the θ_3 term, which leads to an admixture of the Γ_1 order parameter even if T_1 is very small compared with T_5 . So we find for T close to T_5 .

$$|\eta| = \frac{\theta_3}{2A_1(T)} |\eta|^3, \quad (12)$$

with the relative phase

$$\phi \quad \phi \quad \left| \begin{array}{l} 0, \theta_3 < 0 \\ \pi, \theta_3 > 0 \end{array} \right.$$

The Γ_1 component increase respectively to $[T - T_5]^{3/2}$, i.e., a “driven” order parameter. This CR state conserves time – reversal symmetry and is fourfold degenerate $[D_{3d}(\Gamma_1)]$. According to the conditions for an admixture of another representation mentioned there, the actual (Γ_5) state can mix with the (Γ_1) representation, since it has the symmetry $D_{3d}(\Gamma_1)$, compatible with (Γ_1). The CR state maintains the symmetry of the originally classified state (Monien et al. 1986, Wojcanowski and Wolfle, 1986)

3. RESULTS AND DISCUSSION

For lower temperatures an additional second-order phase transition can appear. The only symmetry that can be broken in our restricted free energy is time reversal symmetry, by a change of the relative phase $(\bar{\phi} - \phi)$. Obviously, this is favourable only if $\theta_2 > 0$, since both $\bar{\phi} - \phi = 0$ and $= \pi$ minimize the θ_2 term for $\theta_2 < 0$. Differentiating the free energy with respect to the relative phase, we obtain the extremum condition

$$\sin(\bar{\phi} - \phi)[4\theta_2|\eta| \cos(\bar{\phi} - \phi) + \theta_3|\eta|] = 0 \quad (13)$$

The expression in the brackets gives a temperature dependent solution for $\bar{\phi} - \phi$ only if $\theta_3|\eta|/4\theta_2|\eta| \ll 1$.

Thus a continuous transition from a state with $\bar{\phi} - \phi = 0$ or π takes place at the temperature with T_1 with $|\theta_3||\eta|(T_1) = 4\theta_2|\eta|(T_1)|$. Obviously, for $\theta_2 < 0$ no such transition is possible. Turning to the opposite case, $T_1 > T_5$ we obtain immediately below T_1 the SR (Γ_1) state (equation 7). This leads to an effective free energy for η which contains, in addition to even order terms, a third-order term of the form

$$3\theta(\cos \bar{\phi} - \phi) \left| \frac{-A_4(T)}{2\beta} \right|^{\frac{1}{2}} |\bar{\eta}|^3 \quad 14$$

This term can produce an instability to a CR state through a first-order transition if the coefficients in the free energy satisfy the relation

$$\theta_3 4(\theta_2 + |\theta_2|)[3\beta'_1 + \beta''_2] + \beta'_1 \quad 15$$

Otherwise the transition is continuous. This condition can be derived by the minimization of the free energy with repeat to $|\bar{\eta}|$ for a given η at the transition point or the continuous transition from the SR (Γ_1) to the CR ($\Gamma_1 + \Gamma_5$) state [$A_5(T) - |\eta|^5(\theta_1 - |\theta_2|) = 0$]. If a finite η minimizes the free energy, then a first-order transition has already taken place above this second – order transition point. The symmetry of the CR state is $D_{3d}(\Gamma_1)$ for $\theta_2 < 0$ and $D_{3d}(\Gamma_1 \otimes \Gamma_4)$ for $\theta_2 > 0$. in the latter case there is an additional continuous phase transition possible to the time reversal conserving, state according to (equation 13), but only if the first additional transition was of second order (equation 15) is not satisfied. As in the former example, a series of three continuous transitions is possible here. A more detailed discussion of this example has been given by Lukjanchak and Minreev (1989).

4. CONCLUSION

Finally, we should like to mention that in general the treatment of first-order transition in a multi-component Landau theory is not simple. There is no obvious relation between the high and the low temperature states like the group – theoretical arguments available for second – order phase transitions. The search for the global minimum in a high – dimensional order – parameter space is then more or less a matter of trial and error, whether one uses analytical or numerical methods

5. REFERENCES

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