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Mechanism for Generation of Triplet Superconductivity[†]

Allan I. Solomon[*] and Joseph L. Birman[**]
IHES, Bures-sur-Yvette, France 91440

Abstract

We show, using the relevant dynamical symmetry, that for a system in which singlet superconductivity and charge and spin density waves coexist, a triplet superconductivity operator is spontaneously generated, and has non-zero expectation value in the ground state.

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[†] Reprint requests should be sent to the authors' permanent addresses.

[*] Permanent address: Faculty of Math., Open University, Milton Keynes, UK

[**] Permanent address: Dept. of Physics, City College, CUNY, New York, NY 10031 USA

Coexistence of superconductivity, charge and spin density waves (respectively CDW and SDW) has been recently actively investigated experimentally and theoretically[1,2,3]. In this Letter we show that triplet superconductivity (TS) spontaneously arises in an interacting electron system due to the interplay between singlet superconductivity (SS) and charge and spin density waves (CDW and SDW). Our analysis uses the relevant dynamical symmetry of the model.

Consider a mean-field Hamiltonian $H = H_{KE} + H_{SS} + H_{DW}$ which includes single particle energy, singlet superconductivity, and charge and spin density wave terms, respectively, with:

$$H_{KE} = \sum \varepsilon_k \quad a^\dagger_{k\alpha}\, a_{k\alpha}$$
$$H_{SS} = \sum \Delta^* \, a_{k\uparrow}\, a_{-k\downarrow} \quad + \text{h.c.}$$
$$H_{DW} = \sum \gamma_\mu \, a^\dagger_{k+Q}\, \sigma_\mu \, a_k \quad + \text{h.c.}$$

In the above as usual: $a^\dagger_{k\alpha}$ is the electron creation operator for Bloch state $k\alpha$, with $\alpha = \uparrow$ or $\downarrow$, the one-electron energy ε_k is measured from the Fermi energy, the (BCS) SS parameter Δ, and the CDW and SDW parameters γ_μ are complex; $\mu = 0$ for the CDW; $\mu = 1,2,3$ for the SDW; $2\sigma_\mu = \tau_\mu$ where τ_μ are the Pauli matrices ($\tau_0 = I$). The model (and our results) is independent of dimension, but in a quasi-one-dimensional theory we can take the CDW and SDW wave vector $\underline{Q} = 2\underline{k}_F$, and ignore contributions from $|k| > Q$. The model Hamiltonian is then $H = \sum_{k=0}^{k_F} H(k)$ with

$$H(k) = \varepsilon(k)(a^{\dagger}_{k\alpha}a_{k\alpha} + a^{\dagger}_{-k\alpha}a_{-k\alpha}) + \varepsilon(\bar{k})(a^{\dagger}_{\bar{k}\alpha}a_{\bar{k}\alpha} + a^{\dagger}_{-\bar{k}\alpha}a_{-\bar{k}\alpha})$$

$$+ \Delta^{*}(a_{k\uparrow}a_{-k\downarrow} + a_{\bar{k}\uparrow}a_{-\bar{k}\downarrow} - a_{k\downarrow}a_{-k\uparrow} - a_{\bar{k}\downarrow}a_{-\bar{k}\uparrow}) + h.c.$$

$$+ \gamma_{\mu}(a^{\dagger}_{k\alpha}\sigma^{\alpha\beta}_{\mu}a_{\bar{k}\beta} + a^{\dagger}_{-\bar{k}\alpha}\sigma^{\alpha\beta}_{\mu}a_{-k\beta}) + h.c. \tag{1}$$

and we use $\bar{k} \equiv k-Q$. Only spin zero BCS singlet superconductivity is in (1). We show elsewhere[5] that the operators in (1) close under the Lie algebra SU(8).

A new mechanism for the spontaneous generation of triplet superconductivity is contained in the full Hamiltonian, Eq.(1), but a simplified version will suffice here. Choosing, the SDW amplitude parallel to the $\mu = 3$ axis, the parameters Δ and γ_3 (for SS and SDW respectively) to be real, the CDW parameter γ_0 pure imaginary, and usi the "nesting" condition $\varepsilon(k) + \varepsilon(\bar{k}) = 0$ the algebra reduces to SO(4) $\oplus$ SO(4), giving a simpler model yet with the essential physics.

The simpler Hamiltonian we now use is:

$$H(k) = \varepsilon(a^\dagger_{k\uparrow}a_{k\uparrow} + a^\dagger_{-k\downarrow}a_{-k\downarrow} + a^\dagger_{k\downarrow}a_{k\downarrow} + a^\dagger_{-k\uparrow}\, a_{-k\uparrow})$$

$$- \varepsilon(a^\dagger_{\bar{k}\uparrow}\, a_{\bar{k}\uparrow} + a^\dagger_{-\bar{k}\downarrow}\, a_{-\bar{k}\downarrow} + a^\dagger_{\bar{k}\downarrow}\, a_{\bar{k}\downarrow} + a^\dagger_{-\bar{k}\uparrow}\, a_{-\bar{k}\uparrow})$$

$$- \Delta(a^\dagger_{k\uparrow}a^\dagger_{-k\downarrow} + a^\dagger_{\bar{k}\uparrow}\, a^\dagger_{-\bar{k}\downarrow} - a^\dagger_{k\downarrow}a^\dagger_{-k\uparrow} - a^\dagger_{\bar{k}\downarrow}\, a^\dagger_{-\bar{k}\uparrow}) + \text{h.c.}$$

$$+ \tfrac{1}{2}\, \gamma_3(a^\dagger_{k\uparrow}a_{\bar{k}\uparrow} + a_{-k\downarrow}\, a^\dagger_{-\bar{k}\downarrow} - a^\dagger_{k\downarrow}\, a_{\bar{k}\downarrow} - a_{-k\uparrow}a^\dagger_{-\bar{k}\uparrow}) + \text{h.}$$

$$+ \tfrac{1}{2}\, i\, \gamma_0(a^\dagger_{k\uparrow}a_{\bar{k}\uparrow} - a_{-k\downarrow}a^\dagger_{-\bar{k}\downarrow} + a^\dagger_{k\downarrow}a_{\bar{k}\downarrow} - a_{-k\uparrow}a^\dagger_{-\bar{k}\uparrow}) + \text{h.c}$$

(2)

In the above, $\varepsilon \equiv \varepsilon(k) = -\varepsilon(\bar{k})$. We define operators $\underline{L}^{\alpha}$, $\underline{K}^{\alpha}$ ($\alpha = \uparrow$ or $\downarrow$) as follows:

$$L_3^{\uparrow} = \tfrac{1}{2}(a^{\dagger}_{k\uparrow}a_{k\uparrow} + a^{\dagger}_{-k\downarrow}a_{-k\downarrow} - a^{\dagger}_{\bar{k}\uparrow}a_{\bar{k}\uparrow} - a^{\dagger}_{-\bar{k}\downarrow}a_{-\bar{k}\downarrow})$$

$$L_1^{\uparrow} = \tfrac{1}{2}(a^{\dagger}_{k\uparrow}a^{\dagger}_{-k\downarrow} + a^{\dagger}_{\bar{k}\uparrow}a^{\dagger}_{-\bar{k}\downarrow}) + \text{h.c.}$$

$$K_1^{\uparrow} = \tfrac{1}{2}(a^{\dagger}_{k\uparrow}a_{\bar{k}\uparrow} + a_{-k\downarrow}a^{\dagger}_{-\bar{k}\downarrow}) + \text{h.c.}$$

$$K_2^{\uparrow} = -\tfrac{i}{2}(a^{\dagger}_{k\uparrow}a_{\bar{k}\uparrow} - a_{-k\downarrow}a^{\dagger}_{-\bar{k}\downarrow}) + \text{h.c.}$$

with similar expressions for $\underline{L}^{\downarrow}$, $\underline{K}^{\downarrow}$ with the spins reversed.

Then $H(k)$ takes the form

$$H(k) = H^{\uparrow}(k) + H^{\downarrow}(k) \qquad (3)$$

where

$$H^{\alpha}(k) = \underline{\lambda}^{\alpha}\cdot\underline{L}^{\alpha} + \underline{\kappa}^{\alpha}\cdot\underline{K}^{\alpha}, \qquad (\alpha = \uparrow \text{ or } \downarrow)$$

with

$$\underline{\lambda}^{\uparrow} = (-2\Delta,\ 0,\ 2\varepsilon); \quad \underline{\kappa}^{\uparrow} = (\gamma_3,\ -\gamma_0,\ 0);$$

$$\underline{\lambda}^{\downarrow} = (2\Delta,\ 0,\ 2\varepsilon); \quad \underline{\kappa}^{\downarrow} = (-\gamma_3,\ -\gamma_0,\ 0).$$

Introducing operators $L_2^{\uparrow}$, $K_3^{\uparrow}$ as

$$L_2^{\uparrow} = -\frac{i}{2}(a^{\dagger}_{k\uparrow}a^{\dagger}_{-k\downarrow} - a^{\dagger}_{\bar{k}\uparrow}a^{\dagger}_{-\bar{k}\downarrow}) + \text{h.c.}$$

$$K_3^{\uparrow} = \frac{1}{2}(a^{\dagger}_{k\uparrow}a^{\dagger}_{-\bar{k}\downarrow} - a_{-k\downarrow}a_{\bar{k}\uparrow}) + \text{h.c.}$$

and analogous expressions for $L_2^{\downarrow}$, $K_3^{\downarrow}$, the system of operators $\underline{L}^{\alpha}$, $\underline{K}^{\alpha}$ closes under the commutation relations of SO(4) $\oplus$ SO(4):

$$[L_{\ell}^{\alpha}, L_m^{\beta}] = i\delta^{\alpha\beta}\, e_{\ell mn}\, L_n^{\alpha}$$

$$[L_{\ell}^{\alpha}, K_m^{\beta}] = i\delta^{\alpha\beta}\, e_{\ell mn}\, K_n^{\alpha}$$

$$[K_{\ell}^{\alpha}, K_m^{\beta}] = i\delta^{\alpha\beta}\, e_{\ell mn}\, L_n^{\alpha} \qquad \ell,m,n = 1,2,3$$

It follows immediately, on use of the two invariants $\lambda^2 + \kappa^2$ and $\underline{\lambda}\cdot\underline{\kappa}$ associated with SO(4), that the energy spectrum of the system the values

$$E^{\pm}(k) = \frac{1}{2}[4\varepsilon(k)^2 + \gamma_0^2 + (2\Delta \pm \gamma_3)^2]^{\frac{1}{2}} \quad . \tag{4}$$

Examining[5] the transformation under spin, parity, and time reversal of all the operators in this algebra we note that triplet superconductivity (TS) corresponds to the two operators

$$Q_{TS}^{(1)} \equiv \tfrac{1}{2}(L_1^{\uparrow} + L_1^{\downarrow}) = \frac{1}{4}(a^{\dagger}_{k\uparrow}a^{\dagger}_{-k\downarrow} + a^{\dagger}_{k\downarrow}a^{\dagger}_{-k\uparrow} + (k\to\bar{k})) + \text{h.c.}$$

$$Q_{TS}^{(2)} \equiv \tfrac{1}{2}(L_2^{\uparrow} + L_2^{\downarrow}) = -\frac{i}{4}(a^{\dagger}_{k\uparrow}a^{\dagger}_{-k\downarrow} + a^{\dagger}_{k\downarrow}a^{\dagger}_{-k\uparrow} - (k\to\bar{k})) + \text{h.c.}$$

(5)

But with $\lambda_1^{\uparrow} = -\lambda_1^{\downarrow}$ and $\lambda_2^{\uparrow} = \lambda_2^{\downarrow} = 0$, TS is absent from (3).

We now consider the expectation values of various operators in the ground state $|g\rangle$ of the Hamiltonian (3). For reference note the filled Fermi sea $|f\rangle = \prod_{k=0}^{K_F} a^{\dagger}_{k\uparrow} a^{\dagger}_{k\downarrow} a^{\dagger}_{-k\uparrow} a^{\dagger}_{-k\downarrow} |0\rangle$. We diagonalize (3) by the rotation R, where $R = \prod_k R(k)$, and

$$R(k) = e^{i\phi_2(L_2^{\uparrow}-L_2^{\downarrow})}\, e^{i\phi'_2(K_2^{\uparrow}-K_2^{\downarrow})}\, e^{i\phi_1(K_1^{\uparrow}+K_1^{\downarrow})}$$

with

$$\phi_1 = \tan^{-1}(\gamma_0/2\varepsilon)$$

$$\phi_2 = -(1/2)\tan^{-1}\{4\Delta(4\varepsilon^2+\gamma_0^2)^{\frac{1}{2}}/(4\varepsilon^2+\gamma_0^2+\gamma_3^2-4\Delta^2)\}$$

$$\phi'_2 = (1/2)\tan^{-1}\{2\gamma_3(4\varepsilon^2+\gamma_0^2)^{\frac{1}{2}}/(4\varepsilon^2+\gamma_0^2-\gamma_3^2+4\Delta^2)\} \tag{6}$$

[Index k is suppressed.] The corresponding ground state $|g\rangle$ is then given by $|g\rangle = R^{-1}|f\rangle$. The triplet superconducting order parameter $\langle g|\,Q_{TS}^{(2)}\,|g\rangle$ is evaluated by noting that $\langle f|\,R(L_2^{\uparrow}+L_2^{\downarrow})\,R^{-1}\,|f\rangle = \sin\phi_1\,\sin\phi_2\,\sin\phi_2'\ \langle f|\,L_3^{\uparrow}+L_3^{\downarrow}\,|f\rangle$. So

$$\eta_{TS} \equiv \langle g|Q_{TS}^{(2)}|g\rangle = \sin\phi_1\,\sin\phi_2\,\sin\phi_2' \tag{7}$$

This order parameter is not zero in general; it is enhanced for electrons at the Fermi surface where $\varepsilon = 0$ and $\sin\phi_1 = 1$.

In Table 1 we list all 12 operators Q_A of this model,[6] the type of phase corresponding, transformation under rotation (scalar, vector), time reversal and parity, and the order parameter

$\eta_A \equiv \langle g|Q_A|g\rangle$.

Mechanisms for spontaneous generation of TS emerge when we consider the time evolution of the term in (3) which represents singlet superconductivity: $Q_{SS} \equiv \frac{1}{2}(L_1^{\uparrow}-L_1^{\downarrow})$. Thus

$$Q_{SS}(t) = e^{iHt}\, Q_{SS}\, e^{-iHt}$$

$$= Q_{SS} + it\,[H,Q_{SS}] + \frac{(it)^2}{2}\,[H,[H,Q_{SS}]] + \ldots \tag{8}$$

The second order term $[H,[H,Q_{SS}]]$ includes a term:

$$[[\gamma_3(K_1^{\uparrow}-K_1^{\downarrow}),\ [\gamma_0(K_2^{\uparrow}+K_2^{\downarrow}),\ 1/2\ (L_1^{\uparrow}-L_1^{\downarrow})]]$$

$$= \ 1/2(\gamma_3\gamma_0)\ (L_2^{\uparrow}+L_2^{\downarrow}) = (\gamma_3\gamma_0)\ Q_{TS}^{(2)} \tag{9}$$

Thus the time evolution of the system generates TS. The scenario of equation (9) corresponds to the process illustrated in Figure 1a in which a singlet Cooper pair interacts with a charge density wave, to produce a virtual intermediate anomalous excitation A carrying δnumber = 1, δmomentum = Q, δspin = 0, which in turn interacts with a spin density wave to eliminate the momentum, and give δspin = 1, thus producing a triplet Cooper pair. An alternative allowed process is illustrated in Figure 1b. Here the intermediate virtual excitation B carries δS = 1, δmomentum = 0. However the process illustrated in Figure 1c is forbidden by time reversal invariance since all three excitations at vertex 1 would have odd time reversal parity.

A simple Landau theory can illustrate the stability of the TS phase. Let η_1, η_2, η_3 be one component order parameters each carrying an appropriate transformation: see Table 1: $\eta_1 \sim$ SS; $\eta_2 \sim$ CDW (at+Q); $\eta_3 \sim$ SDW (at-Q). The free energy is

$$F(\eta_1, \eta_2, \eta_3) = a_1\eta_1^2 + b_1\eta_1^4 + a_2\eta_2^2 + b_2\eta_2^4 + a_3\eta_3^2 + b_3\eta_3^4 + d(\eta_1\eta_2\eta_3)^2 + d'(\eta_1\eta_2\eta_3)^4 \quad (10)$$

Taking into account transformations under spin rotation, time reversal and momentum the product $\eta_{TS} \equiv \eta_1\eta_2\eta_3$ acts as a triplet superconductivity order parameter. If the initial state is coexisting SS plus CDW, take $a_1 < 0$, $a_2 < 0$ and a_3, b_3, $d, d' > 0$, so $F(SS, CDW)_{min}$ has $\eta_1 \neq 0$, $\eta_2 \neq 0$, $\eta_3 = 0$ and thus $\eta_{TS} = 0$. Now let d change sign, keeping a_j, b_j, and $d' > 0$. Then with a reasonable choice of $(-d) > 0$, $F(TS)_{min} < F(SS, CDW)_{min}$ or $F(SS, CDW, SDW)_{min}$ where the last two refer to a system with coexisting two or three phases. $F(TS)_{min}$ is the state with $\eta_{TS} \neq 0$. A "phase transition" to TS state can be first order, with the coefficients as given, or second order if initially $a_1, a_2, a_3 < 0$, $b_j > 0$, $d' > 0$ and d changes sign. Of course in a strictly 1-D theory there is no phase transition.[4]

Hence in an interacting electron system where SS, CDW and SDW coexist, a non-zero TS order parameter is spontaneously generated. If triple phase coexistence does not occur, the TS order parameter may appear if the system is in a region where two phases e.g. SS and CDW coexist, near to the SDW instability.[7] Then by a two-step virtual process involving an anomalous singlet superconductivity intermediate state followed by SDW scattering, the TS state can be generated. In effect this produces a transition in spin-space converting singlet to triplet. The analysis of the full SU(8) model, will be given elsewhere.[5]

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Table 1: Physical Properties of Operators in the SO(4) ⊕ SO(4) Model

Operator $2Q_A$	Type of Phase[a)]	Vector/ Scalar	Order parameter[b)] $\eta_A = \langle g\|Q_A\|g\rangle$	Time Rev. T	Parity P
$L_1^{\uparrow}-L_1^{\downarrow}$	SS	S	$\sin\phi_2 \cos\phi_2'$	-1	1
$(L_2^{\uparrow}-L_2^{\downarrow})$	SS	S	0	1	1
$(L_1^{\uparrow}+L_1^{\downarrow})$	TS	V	0	-1	-1
$(L_2^{\uparrow}+L_2^{\downarrow})$	TS	V	$\sin\phi_1 \sin\phi_2 \sin\phi_2'$	1	-1
$(K_2^{\uparrow}+K_2^{\downarrow})$	CDW	S	$\sin\phi_1 \cos\phi_2 \cos\phi_2'$	1	-1
$K_1^{\uparrow}+K_1^{\downarrow}$	CDW	S	0	-1	-1
$K_1^{\uparrow}-K_1^{\downarrow}$	SDW	V	$\cos\phi_2 \sin\phi_2'$	-1	1
$(K_2^{\uparrow}-K_2^{\downarrow})$	SDW	V	0	1	1
$(K_3^{\uparrow}-K_3^{\downarrow})$	AS	S	0	1	-1
$(K_3^{\uparrow}+K_3^{\downarrow})$	AT	V	$-\cos\phi_1 \sin\phi_2 \sin\phi_2'$	1	1
$(L_3^{\uparrow}+L_3^{\downarrow})$	KE	S	$\cos\phi_1 \cos\phi_2 \cos\phi_2'$	1	1
$(L_3^{\uparrow}-L_3^{\downarrow})$	KE	V	0	1	-1

Footnotes to Table 1

a) Meaning of symbols for "type of phase":

TS -Triplet Superconductivity, (Q=0)

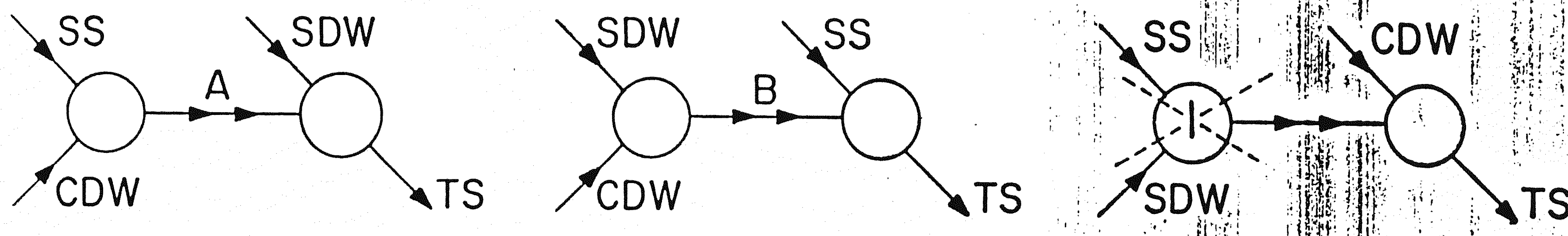
SS -Singlet Superconductivity, (Q=0)

CDW-Charge Density Wave,

SDW-Spin Density Wave,

AS -Anomalous Singlet Superconductivity ($Q\neq 0$)
AT -Anomalous Triplet Superconductivity ($Q\neq 0$)
KE -Kinetic Energy.

b) The definition of angles ϕ_1, ϕ_2, ϕ_2' is given in text.



(a) (b) (c)

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7. In the "g-ology" diagrams in Refs. 4 and 6 such a region is near $g_{2\perp} = - g_{2||} \gtrsim 0$. Likely candidate materials are $NbSe_3$, or $TaSe_3$: near the SS-CDW instability boundary, see Vol. II of Ref.3. We thank Prof. I. Bozović for this suggestion.

Figure Caption

Fig.1 a, b): Allowed processes for TS, c) Forbidden process.