Title	Dynamical Groups and Coexistence of Superconductivity, Charge Density Waves and Magnetism
Creators	Birman, Joseph L. and Solomon, Allan I.
Date	1983
Citation	Birman, Joseph L. and Solomon, Allan I. (1983) Dynamical Groups and Coexistence of Superconductivity, Charge Density Waves and Magnetism. (Preprint)
URL	https://dair.dias.ie/id/eprint/867/
DOI	DIAS-STP-83-18

FM83/A006

DIAS-STP-83-18

Dynamical Groups and Coexistence of Superconductivity, Charge Density Waves and Magnetism

Joseph L. Birman
Physics Department, City College, CUNY, New York,
N.Y., 10031 U.S.A.

and

Allan I. Solomon
Faculty of Mathematics, The Open University,
Milton Keynes, U.K.

Proceedings of the Zvenigorod Conference on Group Theory
Applied in Physics - Nov. 1982. To be published.
(Edited by M.A. Markov and V. Man'ko)

"DYNAMICAL GROUPS AND COEXISTENCE OF SUPERCONDUCTIVITY, CHARGE DENSITY WAVES AND MAGNETISM"

Joseph L. Birman
Physics Department, City College, CUNY, New York, New York 10031 USA

and

Allan I. Solomon
Faculty of Mathematics, The Open University, Milton Keynes, England

Abstract

A summary is given of recent work illustrating the use of dynamical group and algebra concepts in analysis of coexistence of competing many-body effects. The group SU(4) - SO(6) encompasses coexistence of superconductivity, charge density waves and magnetism.

Symmetry-breaking in many-body systems is known to be associated with the appearance of a non-zero expectation value of some order parameter[1]. For example Ferromagnetism breaks the rotational symmetry (broken O(3)) with spontaneous non-zero value of an axial vector. Ferroelectricity breaks O(3) with non-zero value of a polar vector. A not obvious case is superconductivity which breaks SU(2), or "gauge" symmetry. In this connection it is useful to recall a distinction introduced by Wigner[2] between "geometrical" symmetry which relates to the symmetry of the physical domain of the system, versus "dynamical" symmetry which relates to the formal symmetry of the equations of motion for the system.

In the present work we extend the notion of symmetry-breaking to coexisting (or competing) order parameters. We find the dynamical symmetry of the equations of motion and then we demonstrate that different kinds of symmetry-breaking (i.e. different sub-symmetries) correspond to different competing order parameters. We consider below a mean-field Hamiltonian for simultaneous superconductivity, charge density wave, and magnetic order parameters. We find[3] the explicit dynamical group for the Hamiltonian is SU(4). However, we argue the algebraic structure is more general than mean-field approximation.

First we recall the meaning of an order parameter for a material system. Let $\hat{O}$ be some quantum-mechanical operator, whose value $\langle\hat{O}\rangle$ in some state of the system is an observable. If $\langle\hat{O}\rangle = 0$

the system is in a disordered state of high symmetry G. If $\langle \hat{O} \rangle \neq 0$ the system is in an ordered state of broken symmetry $G(\hat{O})$, with $G \subset G(\hat{O})$. We are interested in spontaneous symmetry breaking so $\langle \hat{O} \rangle \neq 0$ with no applied field. Some examples are $\langle \hat{u} \rangle \neq 0$ where $\hat{u}$ is the operator for atom displacement: this is the displacive phase transition; $\langle \hat{M} \rangle \neq 0$ where $\hat{M}$ is the total magnetic moment due to an magnetic ion lattice producing a system magnetization; a spontaneous "band" magnetism could be accounted for by $\langle \hat{\rho}_{\uparrow} - \hat{\rho}_{\downarrow} \rangle \neq 0$ where $\hat{\rho}_{\uparrow}$ is the density operator for band electrons with spin up, and $\hat{\rho}_{\downarrow}$ for those with spin down.

Our question is whether two (or more) operators $\hat{O}_1$ and $\hat{O}_2$ can have non-zero expectation values in the same state: $\langle \hat{O}_1 \rangle \neq 0$, $\langle \hat{O}_2 \rangle \neq 0$. Two examples of competing order parameters relevant to our interest are:

Pair Operator: $a^{\dagger}_{k\uparrow} \, a^{\dagger}_{-k\downarrow} = \hat{O}_1$

with $\langle \hat{O}_1 \rangle \neq 0$ signalling superconductivity;

Charge Density Wave Operator: $a^{\dagger}_{k+Q\uparrow} \, a_{k\uparrow} = \hat{O}_2$

with $\langle \hat{O}_2 \rangle \neq 0$ signalling charge density wave Q is a fixed (external) vector.

The competition between these order parameters can be understood physically beginning with a simple free-electron model. If a Normal → Superconducting transition occurs there will be a gap (2Δ) opened at the (former) Fermi level. This gap can impede the Peierls interaction between electrons which is needed for formation of a charge density wave. In an analogous fashion the existence of magnetic order (i.e. an internal magnetic field due to free-electron band magnetism or to cooperative magnetically ordered sublattice effects) will act to break the Cooper pairs needed for superconductivity. Various microscopic theories have been introduced to investigate these effects.[4] Of overriding significance is that coexistence of superconductivity and charge density wave has been experimentally observed,[5] and also coexistence of superconductivity and magnetism.[6]

A serious limitation of the previous theories is that any symmetry is not manifest, and in fact seems hidden. For this reason inter-alia we examined a mean-field (or reduced) Hamiltonian. The major physical phenomena are known to be describable in terms of this Hamiltonian, although for more quantitative description fluctuations should be added.[4] In the pairing approximation we write H^{RED} as a sum of a "free" part involving single particle band energies ϵ_k, plus a BCS pairing term with SC gap parameter Δ_k, plus a CDW density fluctuation term with a fixed "external" CDW specified by given wave vector Q and CDW gap parameter γ_k. Thus $H^{RED} = H_F + U_{BCS} + U_{CDW}$ where $H_F = \sum_{k,\sigma} \epsilon_k a^\dagger_{k\sigma} a_{k\sigma}$ $(\sigma = \uparrow,\downarrow)$; $U_{BCS} = \sum_k \Lambda_k a_{k\uparrow} a_{-k\downarrow} + h.c.$, and $U_{CDW} = \sum_k \gamma_k a^\dagger_{k+Q,\sigma} a_{k,\sigma} + h.c.$. The Hamiltonian $H_{CDW} = H_F + U_{CDW}$ was treated in reference 7 . Our reduced Hamiltonian is $H^{RED} = \sum_{-k_F}^{k_F} H(k)$

$$H(k) = \epsilon(a^\dagger_{k\uparrow} a_{k\uparrow} + a^\dagger_{-k\downarrow} a_{-k\downarrow}) + \epsilon'(a^\dagger_{k'\uparrow} a_{k'\uparrow} + a^\dagger_{-k'\downarrow} a_{-k'\downarrow})$$
$$+ \gamma a^\dagger_{k\uparrow} a_{k'\uparrow} + \gamma' a^\dagger_{-k'\downarrow} a_{-k\downarrow} + \gamma^* a^\dagger_{k'\uparrow} a_{k\uparrow} + \gamma'^* a^\dagger_{-k\downarrow} a_{-k'\downarrow}$$
$$+ \Lambda a_{k\uparrow} a_{-k\downarrow} + \Lambda' a_{k'\uparrow} a_{-k'\downarrow} + \Lambda^* a^\dagger_{-k\downarrow} a^\dagger_{k\uparrow} + \Lambda'^* a^\dagger_{-k'\downarrow} a^\dagger_{k'\uparrow} \quad (1)$$

Here

$\epsilon = \epsilon_k$, $\epsilon' = \epsilon_{k-Q}$, $\gamma = \gamma_{k-Q}$, $\gamma' = \gamma_{-k}$, $\Lambda = \Lambda_k$, $\Lambda' = \Lambda_{k-Q}$ and

$k' = k-Q$ for $k \in [0, k_F]$;

$\epsilon = \epsilon_k$, $\epsilon' = \epsilon_{k+Q}$, $\gamma = \gamma^*_k$, $\gamma' = \gamma^*_{-(k+Q)}$, $\Lambda = \Lambda_k$, $\Lambda' = \Lambda_{k+Q}$ and

$k' = k+Q$ for $k \in [-k_F, 0]$.

Note $[H(k_1), H(k_2)]_- = 0$.

Define four operators $(A_1, A_2, A_3, A_4) = (a_{k\uparrow}, a^\dagger_{-k\downarrow}, a_{k'\uparrow}, a^\dagger_{-k'\downarrow})$ and form the 16 bilinears: $X_{ij} = A^\dagger_i A_j$ with i, j=1,..., 4. These satisfy the commutation rules of gl(4,R): $[X_{ij}, X_{k\ell}]_- = \delta_{jk} X_{i\ell} - \delta_{i\ell} X_{kj}$. To obtain a matrix representation of H(k) we introduce a standard 4 x 4 matrix basis e_{ij}: $(e_{ij})_{rs} = \delta_{ir} \delta_{js}$ with i,j,r,s=1,...4. These matrices have commutation rules identical to those of the operators X_{ij} and permit us to realize H(k) as 4 x 4 matrix denoted M_k. We introduce five triples of 4 x 4 matrices, fifteeen in all, denoted $\underline{S}$, $\underline{W}$, $\underline{T}$, $\underline{U}$, and $\underline{E}$, where e.g. $\underline{S} \equiv (S_1, S_2, S_3)$ and similarly. Then $2S_i = \tau_0 \times \tau_i$; $2T_i = \tau_1 \times \tau_i$; $2U_i = \tau_2 \times \tau_i$; $2W_i = \tau_3 \times \tau_i$; $2E_i = \tau_i \times \tau_0$, where τ_i (i=1,2,3) are the Pauli matrices and τ_0 the two-dimensional identity matrix. In this basis, H(k) of eqn.(1) is:

$$M_k = \underline{s}_k \cdot \underline{S} + \underline{w}_k \cdot \underline{W} + \underline{e}_k \cdot \underline{E} + \underline{t}_k \cdot \underline{T} + \underline{u}_k \cdot \underline{U}$$

Coefficients in eqn. (2) are given by

$$\underline{s}_k = (-\mathrm{Re}\ (\Delta + \Delta'),\ -\ \mathrm{Im}\ (\Delta + \Delta'),\ \varepsilon + \varepsilon')$$

$$\underline{w}_k = (-\mathrm{Re}\ (\Delta - \Delta'),\ -\ \mathrm{Im}\ (\Delta - \Delta'),\ \varepsilon - \varepsilon')$$

$$\underline{e}_k = (\mathrm{Re}\ (\gamma - \gamma'),\ -\ \mathrm{Im}(\gamma - \gamma'),\ 0)$$

$$\underline{t}_k = (0, 0,\ \mathrm{Re}\ (\gamma + \gamma'))$$

$$\underline{u}_k = (0, 0,\ -\ \mathrm{Im}\ (\gamma + \gamma'))$$

The commutators of the ten matrices $\underline{S}$, $\underline{W}$, E_1, E_2, T_3, U_3 close when augmented by the additional five: E_3, T_m, U_m, $m=1,2$. Hence the dynamical group of M_k, and thus of $H(k)$ is locally SU(4) or SO(6). Note in passing that a Hamiltonian including SC, CDW, and magnetic spin density effects can be expressed, in a mean-field approximation, in a form consistent with SO(6) symmetry. We are investigating this and will report on it elsewhere.[8] The dynamical group of H^{RED} is the direct product of the individual $SO(6)_k$ groups for each k.

Elsewhere we showed[3] that in the physical case for superconductivity plus charge density wave (SC-CDW), $\gamma = \gamma'$, and $\Delta = \Delta' = \Delta^{*}{}'$. Then the effective physical Hamiltonian $H(k)$ is an element in the reduced dynamical group SO(5). It then follows that a unitary operator V_k can be found which transforms

$$H(k) \rightarrow V_k^{\dagger}\ H(k)\ V_k \equiv H'(k) = \lambda_k\ \hat{S}_{3k} + \mu_k\ \hat{W}_{3k}\ .$$

Here λ_k and μ_k are c-numbers. We can express V_k in terms of generators $\hat{L}_{\pm} = \frac{1}{2}(\hat{S}\pm\hat{W})$ in the two SU(2) subalgebras of SO(5). Then

$$V_k = \exp(2i\phi_1 E_2)\ \exp(i\phi_+ L_+/a)\ \exp(i\phi_- L_-/a)$$

where

$$\tan 2\phi_1 = 2\gamma\ (\varepsilon' - \varepsilon)^{-1}\ ,$$

and

$$\tan \phi_{\pm} = 2\Delta[(\varepsilon + \varepsilon') \pm \{(\varepsilon - \varepsilon')^2 + 4\gamma^2\}^{i/2}]^{-1} .$$

Write $T = \prod_k V_k$ as the unitary operator which transforms H_{RED}. Then the eigenstates of H_{RED} can be obtained by operating on those of $\sum H'(k)$ by T. An important eigenstate is the "coherent" ground state $|g>$ of H^{RED} which corresponds to the filled Fermi sea $|f>$. It is:

$$|g> = T\ |f> = T \prod_k a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} |0>$$

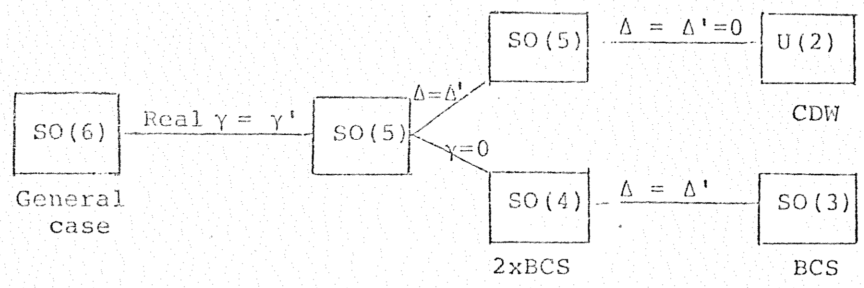
We test for the occurence of superconductivity or charge density waves in state $|g>$ by examining matrix elements $<g|O_1|g>$, and $<g|O_2|g>$ respectively where $O_1 = a^{\dagger}_{k\uparrow}\ a^{\dagger}_{-k\downarrow}$, and $O_2 = a^{\dagger}_{k'\uparrow}\ a_{k\uparrow}$. (Note $k' = k-Q$ for $k \geq 0$, and $k + Q$ for $k < 0$). Using the expression for T we find (with both Δ and γ non-zero):

$$<g|\hat{O}_1|g> = 1/2\ (\cos^2\phi_1\ \sin\ \phi_+ - \sin^2\phi_1\ \sin\ \phi_-) \qquad (A)$$

$$<g|\hat{O}_2|g> = 1/2\ \sin\ 2\phi_1\ \{\sin^2(\phi_-/2) - \cos^2(\phi_+/2) \qquad (B)$$

These expressions give, for each k, the values of the respective order parameters in terms of the Bogoliubov angles. For a given state k we may obtain "phase boundaries" of parameter values between regions of vanishing and non-vanishing order parameters. Thus SC is quenched when (A) vanishes, that is on the hyperbola of parameter values (γ,Δ) $\frac{2\gamma^2}{\varepsilon(\varepsilon' - \varepsilon)} - \frac{\Delta^2}{\varepsilon^2} = 1$ for given k. Similarly the CDW disappears when (B) is zero, on the circle (or hyperbola) $\gamma^2 \pm \Delta^2 = \varepsilon\varepsilon'$.

In Fig. 1 we give a group-subgroup chain illustrating descent in dynamical symmetry from the general SO(6) case, where the parameters Δ, Δ' and γ, γ' are complex and distinct.



Let us now return to consider the problem of coexistent magnetic ordering. If we examine the set of 16 operators $\hat{X}_{ij}$ defined earlier, whose closure defines SU(4) we find amongst them:

$$\text{Antiferromagnetic Pairing} \quad \hat{O}_3 = a^\dagger_{k\uparrow}\, a^\dagger_{k+Q\downarrow}$$

It is natural to consider $\langle\hat{O}_3\rangle \neq 0$ as the signature of Antiferromagnetic (band) ordering. Thus the original algebra contains the possibility of coexistence of two or possibly all three collective phenomena: superconductivity, charge density wave and magnetism. At the time of writing we have not yet obtained the equation of the "phase boundary" for antiferromagnetic order: this is in progress.

A related algebraic approach to coexistence of SC-CDW and magnetism was recently proposed by one of us,[9] and we summarize here. Write 15 generators X_{ij} of SU(4) in the Cartan-Weyl canonical form:

$$SU(4) \rightarrow \{h_1, h_2, h_3;\ e_1, \ldots, e_{12}\}$$

The algebra SU(4) is rank 3 so the three mutually commuting operators are designated h_j. We can identify each of the h_j with a conserved quantity in the disordered phase as

$h_1 \sim \hat{N}$ (number operator)

$h_2 \sim \hat{P}$ (linear momentum)

$h_3 \sim \hat{A}$ ("anomalous" number) .

Now construct the centralizer of h_1, i.e. the subalgebra of all operators commuting with $\hat{N}$. This subalgebra $\mathbb{C}(\hat{N})$ has the structure

$$\mathbb{C}(N) \doteq u(1) \oplus SO(4)$$

where U(1) is the Abelian algebra generated by N and SO(4) $\sim$ (SU(2) x SU(2) is a "charge density wave" subalgebra. We may interpret the elements e_α in this subalgebra as the CDW order parameters. It can be shown that the expectation value of e_α in an eigenstate of the initial Hamiltonian vanishes (i.e. no spontaneous e_α - CDW ordering in the disordered state) while in the ordered state $\langle e_\alpha \rangle \neq 0$. The centralizers $\mathbb{C}$ (P) and $\mathbb{C}$ (A) have been identified with the superconducting and band antiferromagnetic dynamical algebras respectively.[9]

Elsewhere[8] we shall report on the elaboration of a dynamical algebraic formalism to discuss thermal effects and self-consistency as well as selection rules for transition processes.

A major merit of the dynamical algebra approach is that it reveals the underlying group structure of the coexistence problem apart from details of magnitude of the interactions.

This work has been supported in part by grants from PSC-BHE (CUNY Faculty Research Award Program), NSF, and the Research Committee of the Open University. J.L. Birman thanks Prof. M.A. Markov and Prof. V. Man'ko for hospitality and smooth arrangements, and the Academy of Sciences USSR for support during the Conference.

References

1. N. Boccara, "Symmetries Brisśes" Herman et Cie Paris 1978; N. Boccara, (ed) "Symmetries and Broken Symmetries" IDSET, (Paris) (1981).
2. E.P. Wigner "Symmetries and Reflections" U. of Ind. Press, Bloomington, Ind. (1967).
3. J.L. Birman and A.I. Solomon, Phys. Rev. Lett. 49, 230 (1982).
4. K. Levin, D.L. Mills, S.L. Cunningham, Phys. Rev. B10, 3821(1974); G.S. Grest, K. Levin, M.T. Nass, Phys. Rev. B25, 4541, 4562(1962); T.K. Lee, Y.A. Izyumov, J.L. Birman, Phys. Rev. B20, 4494 (1979).

5. R. Sooryakumar and M.V. Klein, Phys. Rev. Lett. 45, 660 (1980) and Phys. Rev. B23, 3213 (1981).

6. See the papers cited in M. Ishikawa, Contemp. Physics 23, 443 (1982).

7. A.I. Solomon and J.L. Birman, Phys. Lett. 88A, 413 (1982).

8. J.L. Birman and A.I. Solomon (to be published).

9. A.I. Solomon (Ann. New York Academy of Science, in press).