The Spectrum-Generating Algebra of the Van Hove Scenario is SO(8)

R.S. Markiewicz1,2 and M.T. Vaughn1
(1) Physics Department and (2) Barnett Institute, Northeastern U., Boston MA 02115

The various nesting and pairing instabilities of the generalized Van Hove scenario can be classified via an SO(8) spectrum-generating algebra. An SO(6) subgroup is an approximate symmetry group of the model, having two 6-dimensional representations (‘superspins’). This group contains as subgroups both the SO(5) and SO(4) groups found by Zhang, while one superspin is a combination of Zhang’s 5-component superspin with a flux phase instability; the other includes a charge density wave instability plus s-wave superconductivity. This is the smallest group which can describe both striped phases and superconductivity.

Two groups play important roles in understanding a Hamiltonian: the symmetry group allows a classification of its degenerate eigenstates, while the Lie group of the spectrum-generating algebra (SGA) can be used to analyze the complete spectrum. SGA’s have proven to be useful in the study of collective modes in nuclear and high-energy physics, while in condensed matter physics they have been used to study phase transitions in liquid He and in one-dimensional (1D) metals. In the 1D metals, the SGA is SU(8), with 63 elements and 56 possible order parameters including superconductivity and charge or spin density (CDW/SDW) waves. This algebra has also been applied to the two-dimensional (2D) Hubbard model. However, we show that even for the generalized Hubbard model appropriate to the generalized Van Hove scenario, the appropriate SGA is SO(8), a considerably smaller algebra. This algebra has a natural subalgebra, SO(6), which acts as an approximate symmetry group generalizing Zhang, and including both his SO(5) and SO(4) as subgroups. We identify SO(6) as the smallest group which is capable of describing striped phases as well as superconductivity.

For a one-dimensional (1D) metal, nesting involves the two points of the Fermi surface, at ±kF, with kF the Fermi momentum. Since this breaks momentum conservation (the states +kF and −kF become inequivalent), the full group SU(8) must be taken as the SGA. On the other hand, in two dimensions, the dominant nesting arises at Q = (π, π), connecting the two Van Hove singularities (VHS’s) at (π, 0) and (0, π). Since the points ±(π, 0) are equivalent points of the reciprocal space lattice, nesting singularities involve only order parameters even in k. Hence the SGA is a proper subgroup of SU(8) – the SO(8) algebra of Table I. (Note that there is some ambiguity in defining a SGA: here we define it as the algebra which contains the mean-field Hamiltonian.)

FIG. 1. Matrix Representation of SO(8), using the shorthand O± = O ± O′.

There is a combinatoric interpretation of this SO(8) which is independent of any particular hamiltonian. Consider an electronic system with a two-fold orbital degeneracy (labelled 1, 2) in addition to the spin degeneracy. The four creation operators can be written as C1↑, C2↑, C1↓, and C2↓. Including both particle-hole (C↓C) and particle-particle (C↑C↑ or CC) operators, there are 28 pair operators, whose components define the Lie algebra of SO(8) [recall that for SO(N), the Lie algebra contains N(N − 1)/2 elements]. Particular linear combinations of these elements are listed in Table I. Figure 1 rewrites these elements as an explicit representation of the Lie algebra of SO(8). The 28 generators are the antisymmetric matrices Lij, with matrix elements Lij = δj i L−j i − δj i L−i j − δj i L−j i L−i j.

$$[L_{ij}, L_{km}] = i(\delta_{ik} L_{jm} + \delta_{jm} L_{ik} - \delta_{im} L_{jk} - \delta_{jk} L_{im}).$$

(1)

SO(8 − M) subalgebras can be formed by eliminating M rows of the L matrices, along with their corresponding columns. These will be designated as \{I1, ..., IM\}, where I1, ..., IM are the rows (and columns) which have been eliminated. For instance, \{234\} is the SO(5) algebra studied by Zhang.

In a generalized Hubbard model, the creation operators can be expanded in terms of operators localized near the corresponding VHS’s:

$$a_{i\sigma}^\dagger \simeq \frac{1}{2}((-1)^x \psi_{1\sigma}^\dagger(\vec{r}) + (-1)^y \psi_{2\sigma}^\dagger(\vec{r})),\quad (2)$$

where \psi_{1\sigma}^\dagger and \psi_{2\sigma}^\dagger are slowly varying functions of position \vec{r} = a(x_i, y_i). A more precise definition is given.
Table I: Generators of SO(8) Lie Algebra

| Operator | Representation |
|----------|----------------|
| $Q$      | $(C_{11}^r C_{11}^l + C_{21}^r C_{21}^l + C_{11}^r C_{11}^l + C_{21}^r C_{21}^l)/2 - 1$ |
| $\tau$  | $(C_{11}^r C_{11}^l - C_{21}^r C_{21}^l + C_{11}^r C_{11}^l - C_{21}^r C_{21}^l)/2$ |
| $S_z$    | $(C_{11}^r C_{11}^l + C_{21}^r C_{21}^l - C_{11}^r C_{11}^l - C_{21}^r C_{21}^l)/2$ |
| $A_x$    | $(C_{11}^r C_{11}^l - C_{21}^r C_{21}^l - C_{11}^r C_{11}^l - C_{21}^r C_{21}^l)/2$ |
| $S_x$    | $(C_{11}^r C_{11}^l + C_{21}^r C_{21}^l - C_{11}^r C_{11}^l + C_{21}^r C_{21}^l)/2$ |
| $A_y$    | $(C_{11}^r C_{11}^l - C_{21}^r C_{21}^l + C_{11}^r C_{11}^l - C_{21}^r C_{21}^l)/2$ |
| $i A_y$  | $(C_{11}^r C_{11}^l + C_{21}^r C_{21}^l + C_{11}^r C_{11}^l + C_{21}^r C_{21}^l)/2$ |
| $O_{SDW}$| $(C_{11}^r C_{21}^l + C_{21}^r C_{11}^l - C_{22}^r C_{22}^l + C_{22}^r C_{22}^l)/2$ |
| $O_{SDW_2}$| $(C_{11}^r C_{21}^l + C_{21}^r C_{11}^l - C_{22}^r C_{22}^l + C_{22}^r C_{22}^l)/2$ |
| $O_{JC}$ | $(C_{11}^r C_{21}^l - C_{21}^r C_{11}^l + C_{22}^r C_{22}^l - C_{22}^r C_{22}^l)/2$ |
| $O_{JSW}$| $(C_{11}^r C_{21}^l - C_{21}^r C_{11}^l - C_{22}^r C_{22}^l - C_{22}^r C_{22}^l)/2$ |
| $i O_{SDW}$| $(C_{11}^r C_{21}^l - C_{21}^r C_{11}^l - C_{22}^r C_{22}^l + C_{22}^r C_{22}^l)/2$ |
| $O_{JSW}$| $(C_{11}^r C_{21}^l - C_{21}^r C_{11}^l + C_{22}^r C_{22}^l - C_{22}^r C_{22}^l)/2$ |
| $i O_{JS}$| $(C_{11}^r C_{21}^l - C_{21}^r C_{11}^l - C_{22}^r C_{22}^l + C_{22}^r C_{22}^l)/2$ |

| Op. | Representation |
|-----|----------------|
| $\Delta_z$ | $(C_{11}^r C_{21}^l + C_{21}^r C_{11}^l)/2$ |
| $\Delta_\phi$ | $(C_{11}^r C_{21}^l + C_{21}^r C_{11}^l)/2$ |
| $-\Pi_y$ | $(C_{21}^r C_{21}^l + C_{21}^r C_{21}^l)/2$ |
| $\Pi_y$ | $(C_{21}^r C_{21}^l - C_{21}^r C_{21}^l)/2$ |
| $\eta$ | $(C_{11}^r C_{21}^l + C_{21}^r C_{11}^l)/2$ |
| $\Pi_z$ | $(C_{11}^r C_{21}^l - C_{21}^r C_{11}^l)/2$ |

Table II: Interaction Terms

- $(G_2 - G_3) \Sigma \tau \Delta_y(\vec{r}) \Delta_y(\vec{r})$
- $(G_2 + G_3) \Sigma \tau \Delta(\vec{r}) \Delta(\vec{r})$
- $(2G_1 + G_3 - G_4) \Sigma \tau O_{CDW}(\vec{r})$
- $(G_3 + G_4 - 2G_1) \Sigma \tau O_{JC}(\vec{r})$
- $(G_4 - G_3) \Sigma \tau O_{JSW}(\vec{r}) \cdot O_{JSW}(\vec{r})$
- $- (G_3 + G_4) \Sigma \tau O_{SDW}(\vec{r}) \cdot O_{SDW}(\vec{r})$

The Lie algebra of Table I corresponds to $O \to \Sigma \tau O(\vec{r})$, with $\Sigma_{\tau_{\pi}} \to \psi_{\tau_{\pi}}(\vec{r})$, etc. With this definition, the operators become equivalent to those introduced by Schulz and Zhang. The SGA $G$ is defined in Fourier space as $G = \oplus \mathfrak{g}^k$, where $\mathfrak{g}^k$ is the algebra of a particular $\vec{k}$-component of the Fourier transformed operators of Table I.

The interaction terms in the generalized Hubbard hamiltonian $H$ can be written in terms of pairs of these operators, Table II. Here the $G_i$’s are coupling constants, which can be related to the Hubbard $U$ and to various near-neighbor interaction terms. For the pure Hubbard model, $G_1 = G_2 = G_3 = G_4$ and $t$ is the nearest neighbor hopping parameter. The form of the interaction term is not unique, since a number of alternative terms can arise by anticommuting the operators.

While SO(8) is the SGA of the generalized Hubbard model, Zhang’s SO(5) is an (approximate) symmetry algebra of the same model – in particular, the collective modes (SDW and d-wave superconductivity for SO(5)) are *elements* of the SGA, but are *components* of a super-spin, which transforms under the symmetry group. For the generalized Hubbard model, the natural (approximate) symmetry group is SO(6), defined as follows. SO(8) contains an SO(3) algebra, which we call isospin, generated by $T_0 = \tau, T_{\pm} = O_{CDW} \pm O_{JC}$. This algebra is the algebra of the VHS’s: the $z$-component of the isospin, $T_0$, measures the excess population of the 1-VHS over the 0-VHS. Those operators which do not commute with $T_0$ can lead to a nesting or pairing instability. Hence, the important transformation group of the VHS’s is the SO(6) subgroup \{23\} which commutes with $T_0$, leading to the decomposition scheme:

\[
\text{SO}(8) \to \text{SO}(6)_{\{23\}} \oplus \mathbf{V}_+ \oplus \mathbf{V}_- \oplus \tau,
\]

under which $28 \to (15, 0) + (6, 1) + (6, -1) + (1, 0)$, where \((m, n)\) denotes representation \(m\) of SO(6) and eigenvalue \(n\) of \(T_0\). The 6-vectors can be denoted $\mathbf{V}_\pm = \mathbf{V} \pm \mathbf{V}'$ with

- $\mathbf{V} = \{L_{21}, L_{42}, L_{52}, L_{62}, L_{72}, L_{82}\}$
- $\mathbf{V}' = \{L_{31}, L_{43}, L_{53}, L_{63}, L_{73}, L_{83}\}$,
A number of points should be noted. (1) The $SO(6)$ group \{23\} contains Zhang’s $SO(5)$ group as a subgroup, as well as the the $SO(4)$ group introduced by Yang and Zhang.\[11\] Moreover, $V^\prime$, Fig. 3 combines Zhang’s $SO(5)$ superspin with $O_{JC}$, which is essentially equivalent to the flux phase.\[14\]

(2) The twelve components of superspin are precisely the collective modes identified earlier by Schulz, and most of them have been found to play an important role in the cuprates: s-wave superconductivity in electron-doped and (possibly) overdoped cuprates, CDW’s near optimal doping,\[6]\[10\] the flux phase\[11\], and the pseudospin degeneracy of one part of the generalized Hubbard hamiltonian,\[17\] the flux phase\[11\] (also a 12-vector) which couples to the superspin with $O_{JC}$, which is essentially equivalent to the flux phase.\[14\]

(3) For a bare band dispersion (neglecting interactions) of the form

$$\epsilon_{\vec{k}} = -2t(\cos k_x a + \cos k_y a) + 4t' \cos k_x a \cos k_y a,$$  \hspace{1cm} (5)

two parameters control the symmetry of the quadratic part of the generalized Hubbard hamiltonian, $t'$ and $\tilde{\mu} = E_F - E_V$, the shift of the Fermi level $E_F$ from the VHS $E_V$. When both parameters are zero (half filling with square Fermi surface) the hamiltonian has an extra pseudospin symmetry.\[17\] In this case, the nature of the ground state instability is controlled solely by the interaction terms (the $G$’s). A pure Hubbard interaction ($U$) breaks the $SO(6)$ symmetry (Table II):

$$SO(6) \rightarrow SO(3) \oplus SO(3),$$  \hspace{1cm} (6)

with one $SO(3)$ ordinary spin, and the other the pseudospin. Both 6-vectors are broken down to pairs of 3-vectors

$$V \rightarrow \{O_{JSI}\} \oplus \{\Delta_s^+ \Delta_s, O_{CDW}\}$$

$$V^\prime \rightarrow \{O_{SDW}\} \oplus \{\Delta_s^+ \Delta_s, O_{JC}\};$$ \hspace{1cm} (7)

however, there remains an accidental degeneracy of one vector ($O_{JSI}$) with the opposite pseudovector. At half filling the lowest energy state is $O_{SDW}$. As discussed below, this weak coupling result must be corrected for strong correlation effects.

When the Fermi surface is distorted from square, either by doping away from half filling ($\tilde{\mu}$) or by introducing second-neighbor hopping terms $t''$, the pseudospin degeneracy is broken, in such a way as to favor pairing over nesting instabilities. This can be seen by Hartree-Fock\[6\] or renormalization group\[10\] analyses or by a linear response analysis (following Ref14).

If the superspin is written as $\tilde{O}$ (a twelve component vector incorporating both representations), then in linear response theory it is assumed that there is an applied field $\vec{h}_O$ (also a 12-vector) which couples to $\tilde{O}$. The hamiltonian in the presence of $\vec{h}_O$ is

$$H = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}\sigma} a_{\vec{k}\sigma}^\dagger a_{\vec{k}\sigma} + \vec{h}_O \cdot \tilde{O},$$  \hspace{1cm} (8)

(here the terms in $G$ have been neglected), with resulting free energy

$$F_{HF}(\vec{O}) = \Omega_0(\mu, \vec{O}, T) + \mu N$$

$$\Omega_0(\mu, \vec{O}, T) = -2kB T \sum_{\vec{k}\sigma} \ln(1 + e^{-\frac{(\epsilon_{\vec{k}\sigma} - \mu)kB T}{T}})$$

$$+ \vec{h}_O \cdot \vec{O},$$  \hspace{1cm} (9)

with $E_{\vec{k}\sigma}$ the quasiparticle energy found by applying a Bogoliubov-Valentin transformation to Eq. 8 or via SGA techniques.\[14\] The expectation value of each superspin component $O_i$ is found from

$$\frac{\partial \Omega_0}{\partial h_{Oi}} = 0,$$  \hspace{1cm} (10)

and the corresponding susceptibility is

$$\chi_{0i} = \lim_{\vec{h}_O \rightarrow 0} \frac{\Omega_{i}}{\vec{h}_O}.$$  \hspace{1cm} (11)

Including the interaction terms, the Hartree-Fock free energy becomes

$$F_{HF}(\vec{O}) = \sum_{i} \left( \frac{1}{2\chi_{0i}} + G_i \right) O_i^2,$$  \hspace{1cm} (12)

leading to an instability of the $i$th mode when

$$1 + 2\chi_{0i} G_i = 0.$$  \hspace{1cm} (13)

If the quadratic hamiltonian is symmetric under $SO(6)$, then the component with the most negative $G_i$ is the first to diverge. For finite $\tilde{\mu}$ or $t''$, the hamiltonian still preserves particle number, so there are only two independent susceptibilities, the particle-hole susceptibility $\chi_{00}$ and the pair susceptibility $\chi_{02}$, with

$$\chi_{00} = -2\sum_{\vec{k}\sigma} \frac{f(\epsilon_{\vec{k}\sigma})}{\epsilon_{\vec{k}\sigma} - \epsilon_{\vec{k}+\vec{Q},\sigma}} \epsilon_{\vec{k}\sigma},$$

$$\chi_{02} = -2\sum_{\vec{k}\sigma} \frac{f(\epsilon_{\vec{k}\sigma})}{\epsilon_{\vec{k}\sigma} - \epsilon_{\vec{k},\sigma} - \epsilon_{\vec{F}}}. $$  \hspace{1cm} (14)

Note that in nearest-neighbor hopping models ($t'' = 0$) $\epsilon_{\vec{k}+\vec{Q},\sigma} = -\epsilon_{\vec{k},\sigma}$, and the two expressions become equivalent when $\epsilon_{\vec{F}} = 0$ i.e., at half filling.

Figure 3 illustrates the doping dependence of these susceptibilities for a Hubbard band with nearest-neighbor hopping only ($t'' = 0$). The point of maximum instability (largest $\chi$) coincides with the point at which the VHS

FIG. 3. Susceptibilities $\chi_{00}$ (dotdashed line) and $\chi_{02}$ (solid line) vs. band filling $1 + x$ for Eq. 12 with $t'' = 0$.  \hspace{1cm} 3
crosses the Fermi level – half filling when \( t' = 0 \). When \( x = t' = 0 \), the susceptibilities are degenerate, \( \chi_{00} = \chi_{02} \), as expected from the pseudospin symmetry. However, as soon as the system is doped away from half filling (\( x \neq 0 \)) the electron-hole susceptibility drops precipitously, whereas the pair susceptibility falls off much more gradually. A similar effect arises if the system is maintained at optimal doping (the VHS), but the parameter \( t' \) is varied – indeed \( \chi_{02} \) actually increases with increasing \( t' \), Fig 3. This striking difference is readily understood: the electron-hole susceptibility involves inter-VHS nesting, which gets progressively worse as the Fermi surface gets more curved, whereas the electron-electron susceptibility involves intra-VHS scattering, and increases with \( t' \) as the Fermi surfaces become nearly 1D near the VHS’s. (In Figs. 3 and 4, the logarithmic divergence at the VHS was cut off by adding a small imaginary term to the denominator of \( \chi \).)

![Graph 4](image)

**FIG. 4.** As in Fig. 3, but with \( 4t' = E_F \).

Figure 3 is consistent with the RG results of Schulz. From Eq. 13, when all \( \chi's \) are equal the order parameter associated with the most negative \( G \) is the first to go singular. For the pure Hubbard model, this means that the leading instability at half filling is the SDW. When the material is doped, the SDW susceptibility plummets, and at some point d-wave superconductivity becomes favorable. In agreement with Zhang, the shift of the Fermi energy from the VHS is a relevant parameter in driving this SDW→ d-wave superconducting transition.

Despite the simplicity of this picture, a purely SO(5) model cannot explain the full physics of the cuprates. First, the above analysis is in the weak coupling limit, and a strong coupling reanalysis of Table II (J-term dominant) shows that the flux phase – not included in SO(5) – is the lowest energy state. A second problem is in \( \text{La}_{2-x}\text{Ba}_x\text{CuO}_4 \) and \( \text{La}_{2-x-y}\text{Nd}_y\text{Sr}_x\text{CuO}_4 \), near \( x = 1/8 \), where the striped phase is commensurately pinned, leading to long-ranged magnetic and charge order. At the same time, superconductivity is strongly suppressed, demonstrating that whatever the driving force for charge order may be, it is not superconductivity, but is in competition with superconductivity. Since SO(5) only allows for antiferromagnetism and superconductivity, it does not have sufficient flexibility to properly describe this situation. There are strong hints that the charged stripes are associated with a CDW: the low-temperature tetragonal phase is nearly coterminal with the long-range SDW-ordered phase, and the fact that the charged stripes are best seen by neutron diffraction suggests a strong associated lattice distortion. There is considerable additional evidence that phonons and structural instabilities play an important role in the doped material. Hence, for a detailed description of the doping dependence of the pseudogap, striped phases, and extended VHS’s, it may be necessary to recognize that strong electron-phonon coupling can lead to a crossover to a groundstate involving the 6-vector.

MTV’s research is supported by the Dept. of Energy under Grant # DE-FG02-85ER40233. Publication 722 of the Barnett Institute.

1 “Dynamical Groups and Spectrum Generating Algebras”, ed. by A. Bohm, Y. Ne’eman, and A.O. Barut (Singapore, World Scientific, 1988).
2 A.I. Solomon and J.L. Birman, J. Math. Phys. 28, 1526 (1987).
3 A.B. Eriksson, T. Einarsson, and S. Östlund, Phys. Rev. B52, 3662 (1995).
4 S.-C. Zhang, Science 275, 1089 (1997).
5 J. Sölyom, Adv. Phys. 28, 201 (1979).
6 T.M. Rice and G.K. Scott, Phys. Rev. Lett. 35, 120 (1975).
7 H.J. Schulz, Phys. Rev. B39, 2940 (1989).
8 R.S. Markiewicz, Physica C210, 235 (1993).
9 R.S. Markiewicz and M.T. Vaughan, to be published, J. Phys. Chem. Sol. cond-mat/9709137, and unpublished.
10 C.N. Yang and S.-C. Zhang, Mod. Phys. Lett. B4, 759 (1990); S.-C. Zhang, Phys. Rev. Lett. 65, 120 (1990).
11 I. Affleck and J.B.Marston, Phys. Rev. B37, 3774 (1988).
12 R.S. Markiewicz, J. Phys. Chem. Sol. 58, 1179 (1997).
13 R.S. Markiewicz, Phys. Rev. B56, 9901, (1997).
14 T.C. Hsu, Phys. Rev. B41, 11379 (1990); R.B. Laughlin, J. Phys. Chem. Sol. 56, 1627 (1995); X.-G. Wen and P.A. Lee, Phys. Rev. Lett. 76, 503 (1996).
15 C.A. Balseiro and L.M. Falicov, Phys. Rev. B20, 4457 (1979).
16 I. E. Dzyaloshinskii, Zh. Eksp. Teor. Fiz. 93, 1487 (1987) [Sov. Phys.-JETP 66, 848 (1987)].
17 H. Schulz, Europhys. Lett. 4, 609 (1987).
18 T. Moriya, “Spin Fluctuations in Itinerant Electron Magnetism” (Springer, Berlin, 1985).
19 J.M. Tranquada, B.J. Sternlieb, J.D. Axe, Y. Nakamura, and S. Uchida, Nature 375, 561 (1995); J.M. Tranquada, J.D. Axe, N. Ichikawa, A.R. Moodenbaugh, Y. Nakamura, and S. Uchida, Phys. Rev. Lett 78, 338 (1997).