Classification of the Van Hove scenario as an SO(8) spectrum-generating algebra

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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 six-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 five-component superspin with a flux phase instability; the other includes a charge-density-wave instability plus *s*-wave superconductivity. This is the smallest group that can describe both striped phases and superconductivity. [S0163-1829(98)52322-3]

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 algebra¹ (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 onedimensional (1D) metals.² 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.³ 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,⁴ 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,⁵ nesting involves the two points of the Fermi surface, at $\pm k_F$, with k_F the Fermi momentum. Since this breaks momentum conservation (the states $+k_F$ and $-k_F$ become inequivalent), the *full group* SU(8) must be taken as the SGA.² On the other hand, in two dimensions, the dominant nesting arises at $\vec{Q} = (\pi, \pi)$, connecting the two Van Hove singularities (VHS's) (Ref. 6) at $(\pi,0)$ and $(0,\pi)$. Since the points $\pm(\pi,0)$ are equivalent points of the reciprocal space lattice, nesting singularities involve only order parameters even in \vec{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.)

There is a combinatoric interpretation of this SO(8) which is independent of any particular Hamiltonian. Consider an electronic system with a twofold orbital degeneracy (labeled 1, 2) in addition to the spin degeneracy. The four creation operators can be written as $C_{1\uparrow}^{\dagger}$, $C_{2\uparrow}^{\dagger}$, $C_{1\downarrow}^{\dagger}$, and $C_{2\downarrow}^{\dagger}$. Including both particle-hole ($C^{\dagger}C$) and particle-particle ($C^{\dagger}C^{\dagger}$ 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 L^{ij} , with matrix elements $L_{kl}^{ij} = \delta_k^i \delta_l^j$

TABLE I. Generators of SO(8) Lie algebra.

Operator	Representation						
Q	$(C_{1\uparrow}^{\dagger}C_{1\uparrow}+C_{1}+C_{1}$	$C_{2\uparrow}^{\dagger}C_{2\uparrow}+$	$C_{1\downarrow}^{\dagger}C_{1\downarrow} + C_{2\downarrow}^{\dagger}C_{2\downarrow})/2 - 1$				
au			$+C_{1\downarrow}^{\dagger}C_{1\downarrow}-C_{2\downarrow}^{\dagger}C_{2\downarrow})/2$				
S_z			$-C_{1\downarrow}^{\dagger}C_{1\downarrow}-C_{2\downarrow}^{\dagger}C_{2\downarrow})/2$				
A_z			$-C_{1\downarrow}^{\dagger}C_{1\downarrow}+C_{2\downarrow}^{\dagger}C_{2\downarrow})/2$				
S_x			$+C_{1\downarrow}^{\dagger}C_{1\uparrow}+C_{2\downarrow}^{\dagger}C_{2\uparrow})/2$				
A_x			$+C_{1\downarrow}^{\dagger}C_{1\uparrow}-C_{2\downarrow}^{\dagger}C_{2\uparrow})/2$				
iS_y			$-C_{1\downarrow}^{\dagger}C_{1\uparrow}-C_{2\downarrow}^{\dagger}C_{2\uparrow})/2$				
iA_y			$-C_{1\downarrow}^{\dagger}C_{1\uparrow}+C_{2\downarrow}^{\dagger}C_{2\uparrow})/2$				
O_{CDW}			$+C_{1\downarrow}^{\dagger}C_{2\downarrow}+C_{2\downarrow}^{\dagger}C_{1\downarrow})/2$				
O_{SDWz}			$-C_{1\downarrow}^{\dagger}C_{2\downarrow}-C_{2\downarrow}^{\dagger}C_{1\downarrow})/2$				
O_{JC}			$+C_{1\downarrow}^{\dagger}C_{2\downarrow}-C_{2\downarrow}^{\dagger}C_{1\downarrow})/2$				
O_{JSz}			$-C_{1\downarrow}^{\dagger}C_{2\downarrow}+C_{2\downarrow}^{\dagger}C_{1\downarrow})/2$				
O_{SDWx}			$+C_{1\downarrow}^{\dagger}C_{2\uparrow}+C_{2\downarrow}^{\dagger}C_{1\uparrow})/2$				
<i>iO_{SDWy}</i>			$-C_{1\downarrow}^{\dagger}C_{2\uparrow}-C_{2\downarrow}^{\dagger}C_{1\uparrow})/2$				
O_{JSx}			$+C_{1\downarrow}^{\dagger}C_{2\uparrow}-C_{2\downarrow}^{\dagger}C_{1\uparrow})/2$				
<i>iO</i> _{JSy}	$(C_{1\uparrow}^{\dagger}C_{2\downarrow}^{}$	$-C_{2\uparrow}C_{1\downarrow}$	$-C_{1\downarrow}^{\dagger}C_{2\uparrow}+C_{2\downarrow}^{\dagger}C_{1\uparrow})/2$				
Op.	Representation	Op.	Representation				
Δ_s	$(C_{1\uparrow}C_{1\downarrow}+C_{2\uparrow}C_{2\downarrow})/2$	Δ_s^\dagger	$(C_{1\downarrow}^{\dagger}C_{1\uparrow}^{\dagger}+C_{2\downarrow}^{\dagger}C_{2\uparrow}^{\dagger})/2$				
Δ_d	$(C_{1\uparrow}C_{1\downarrow} - C_{2\uparrow}C_{2\downarrow})/2$	Δ_d^\dagger	$(C_{1\downarrow}^{\dagger}C_{1\uparrow}^{\dagger}-C_{2\downarrow}^{\dagger}C_{2\uparrow}^{\dagger})/2$				
$-i\Pi_y$	$(C_{2\uparrow}C_{1\uparrow}+C_{2\downarrow}C_{1\downarrow})/2$	$i\Pi_y^\dagger$	$(C_{1\uparrow}^{\dagger}C_{2\uparrow}^{\dagger}+C_{1\downarrow}^{\dagger}C_{2\downarrow}^{\dagger})/2$				
Π_x	$(C_{2\uparrow}C_{1\uparrow} - C_{2\downarrow}C_{1\downarrow})/2$	Π_x^{\dagger}	$(C_{1\uparrow}^{\dagger}C_{2\uparrow}^{\dagger}-C_{1\downarrow}^{\dagger}C_{2\downarrow}^{\dagger})/2$				
η	$(C_{1\uparrow}C_{2\downarrow}+C_{2\uparrow}C_{1\downarrow})/2$	η^{\dagger}	$(C_{2\downarrow}^{\dagger}C_{1\uparrow}^{\dagger}+C_{1\downarrow}^{\dagger}C_{2\uparrow}^{\dagger})/2$				
Π_z	$(C_{1\uparrow}C_{2\downarrow} - C_{2\uparrow}C_{1\downarrow})/2$	Π_z^\dagger	$(C_{2\downarrow}^{\dagger}C_{1\uparrow}^{\dagger}-C_{1\downarrow}^{\dagger}C_{2\uparrow}^{\dagger})/2$				

<u>57</u>

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Δ_s^+		_				
$-i\Delta_d^-$	au		_			
$-i\eta^-$	O_{CDW}	iO_{JC}		_		
Π_x^+	$-iO_{JSx}$	O_{SDWx}	$-A_x$		_	
Π_y^+	$-iO_{JSy}$	$O_{SDW \boldsymbol{y}}$	$-A_y$	$-S_z$		_
Π_z^+	$-iO_{JSz}$	O_{SDWz}	$-A_z$	S_y	$-S_x$	
Q	$i\Delta_s^-$	Δ_d^+	η^+	$i\Pi_x^-$	$i\Pi_y^-$	$i\Pi_z^-$

FIG. 1. Matrix representation of SO(8), using the shorthand $O_{\pm} = O \pm O^{\dagger}$.

 $-\delta_l^i \delta_k^j$. Figure 1 illustrates the equivalences as the lower half of an antisymmetric *L* matrix. The operators satisfy the Lie algebra, with standard SO(8) commutation rules:

$$[L^{ij}, L^{km}] = i(\delta_{ik}L^{jm} + \delta_{jm}L^{ik} - \delta_{im}L^{jk} - \delta_{jk}L^{im}).$$
(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 $\{I_1, \ldots, I_M\}$, where I_1, \ldots, I_M are the rows (and columns) which have been eliminated. For instance, $\{234\}$ is the SO(5) algebra studied by Zhang.⁴

In a generalized Hubbard model,⁷ the creation operators can be expanded in terms of operators localized near the corresponding VHS's:

$$a_{i\sigma}^{\dagger} \approx \frac{1}{2} [(-1)^{x_i} \psi_{1\sigma}^{\dagger}(\vec{r}) + (-1)^{y_i} \psi_{2\sigma}^{\dagger}(\vec{r})], \qquad (2)$$

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 in Refs. 8 and 9. The Lie algebra of Table I corresponds to $O \rightarrow \sum_{\vec{r}} O(\vec{r})$, with $C_{i\sigma}^{\dagger} \rightarrow \psi_{i\sigma}^{\dagger}(\vec{r})$, etc. With this definition, the operators become equivalent to those introduced by Schulz⁷ and Zhang.⁴ The SGA **G** is defined in Fourier space as **G** $= \bigoplus_{\vec{k}} \mathbf{g}_{\vec{k}}$, where $\mathbf{g}_{\vec{k}}$ is the algebra of a particular \vec{k} component of the Fourier transformed operators of Table I.

The interaction terms in the generalized Hubbard Hamiltonian⁷ can be written in terms of pairs of these operators; see 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.⁷ For the pure Hubbard model, $G_1 = G_2 = G_3 = G_4 = U/4\pi t$ and t is the nearest-neighbor

TABLE II. Interaction terms.

$(G_2 - G_3) \Sigma_{\vec{r}} \Delta_d^{\dagger}(\vec{r}) \Delta_d(\vec{r})$	
$(G_2 + G_3) \Sigma_{\vec{r}} \Delta_s^{\dagger}(\vec{r}) \Delta_s(\vec{r})$	
$(2G_1 + G_3 - G_4) \Sigma_{\vec{r}} [O_{CDW}(\vec{r})]^2$	
$(G_3 + G_4 - 2G_1) \Sigma_{\vec{r}} [O_{JC}(\vec{r})]^2$	
$(G_4 - G_3) \Sigma_{\vec{r}} \vec{O}_{JS}(\vec{r}) \cdot \vec{O}_{JS}(\vec{r})$	
$-(G_3+G_4)\Sigma_{\vec{r}}\vec{O}_{SDW}(\vec{r})\cdot\vec{O}_{SDW}(\vec{r})$	

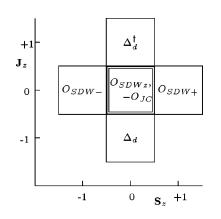


FIG. 2. SO(4) weight diagram of \mathbf{V}' , where S_z (J_z) is the z component of spin (pseudospin).

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 superspin, 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 2 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:

$$\mathbf{SO(8)} \rightarrow \mathbf{SO(6)}_{\{23\}} \oplus \mathbf{V}_{+} \oplus \mathbf{V}_{-} \oplus \tau, \tag{3}$$

under which $28 \rightarrow (15,0) + (6,1) + (6,-1) + (1,0)$, where (\mathbf{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

$$\mathbf{V} = \{L_{21}, L_{42}, L_{52}, L_{62}, L_{72}, L_{82}\}$$
$$\mathbf{V}' = \{L_{31}, L_{43}, L_{53}, L_{63}, L_{73}, L_{83}\},$$
(4)

shown boxed in Fig. 1. The group structure of **V**' is shown in Fig. 2, where J_z is the *z* component of the pseudospin operator introduced by Yang and Zhang¹⁰ and $O_{SDW\pm} = \mp (O_{SDWx} \pm i O_{SDWy})/\sqrt{2}$. An analogous diagram can be drawn for **V**. The group SO(6)_{23} transforms the components of each of these 6-vectors among themselves, without mixing the two vectors, while τ transforms the vectors into each other.

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 SO(4) group introduced by Yang and Zhang.¹⁰ Moreover, **V**', Fig. 2, combines Zhang's SO(5) superspin with O_{JC} , which is essentially equivalent to the flux phase.¹¹

(2) The 12 components of superspin are precisely the collective modes identified earlier by Schulz,⁷ 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,^{12,13} the flux phase near half filling.^{14,13}

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

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

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.¹⁰ 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):

$$SO(6) \rightarrow SO(3) \oplus SO(3),$$
 (6)

with one SO(3) ordinary spin, and the other the pseudospin.¹⁰ Both 6-vectors are broken down to pairs of 3-vectors

$$\mathbf{V} \rightarrow \{\mathbf{O}_{\mathbf{J}\mathbf{S}\mathbf{i}}\} \oplus \{\mathbf{\Delta}_{\mathbf{s}}^{\dagger}, \mathbf{\Delta}_{\mathbf{s}}, \mathbf{O}_{CDW}\}$$
$$\mathbf{V}' \rightarrow \{\mathbf{O}_{\mathbf{S}\mathbf{D}\mathbf{W}\mathbf{i}}\} \oplus \{\mathbf{\Delta}_{\mathbf{d}}^{\dagger}, \mathbf{\Delta}_{\mathbf{d}}, \mathbf{O}_{\mathbf{J}\mathbf{C}}\};$$
(7)

however, there remains an accidental degeneracy of one vector (O_{JS}) 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 secondneighbor 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-Fock¹⁵ or renormalization group^{16,17,12} analyses or by a linear response analysis (following Ref. 18).

If the superspin is written as \vec{O} (a 12-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 \vec{O} . The Hamiltonian in the presence of \vec{h}_O is

$$H = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} a^{\dagger}_{\vec{k}\sigma} a_{\vec{k}\sigma} + \vec{h}_{O} \cdot \vec{O}$$
(8)

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

$$F_{0}(\vec{O}) = \Omega_{0}(\mu, \vec{O}, T) + \mu N,$$

$$\Omega_{0}(\mu, \vec{O}, T) = -2k_{B}T\Sigma_{\vec{k}\sigma} \ln(1 + e^{-(E_{\vec{k}\sigma}^{-} - \mu)/k_{B}T}) + \vec{h}_{O} \cdot \vec{O},$$
(9)

with $E_{\vec{k}\sigma}$ the quasiparticle energy found by applying a Bogoliubov-Valentin transformation to Eq. (8) or via SGA techniques.^{1,2} The expectation value of each superspin component O_i is found from

$$\frac{\partial \Omega_0}{\partial h_{Oi}} = 0, \tag{10}$$

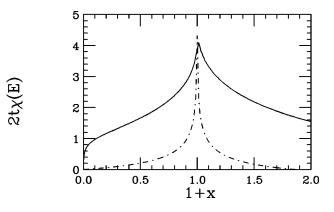


FIG. 3. Susceptibilities χ_{00} (dot-dashed line) and χ_{02} (solid line) vs band filling 1 + x for Eq. (5) with t' = 0.

and the corresponding susceptibility is

$$\chi_{0i} = \lim_{\vec{h}_O \to 0} \left(\frac{O_i}{h_{Oi}} \right). \tag{11}$$

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

$$F_{HF}(\vec{O}) = \sum_{i} \left(\frac{1}{2\chi_{0i}} + G_{i} \right) O_{i}^{2}, \qquad (12)$$

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

$$1 + 2\chi_{0i}G_i = 0.$$
 (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 χ_{00} and the pair susceptibility χ_{02} , with

$$\chi_{00} = -2\Sigma_{\vec{k}\sigma} \frac{f(\epsilon_{\vec{k}\sigma})}{\epsilon_{\vec{k}\sigma} - \epsilon_{\vec{k}} + \bar{\varrho}_{,\sigma}},$$

$$\chi_{02} = -\Sigma_{\vec{k}\sigma} \frac{f(\epsilon_{\vec{k}\sigma})}{\epsilon_{\vec{k}\sigma} - \epsilon_{F}}.$$
(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 $\epsilon_F = 0$, 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 χ) coincides with the point at which the VHS 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.¹⁰ 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 χ_{02} actually increases with increasing t' (Fig. 4). This striking difference is readily understood: the electron-hole susceptibility involves inter-

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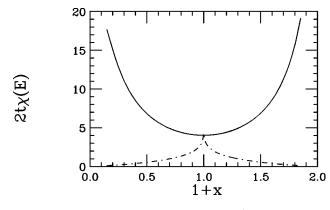


FIG. 4. As in Fig. 3, but with $4t' = E_F$.

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 χ .)

Figure 3 is consistent with the RG results of Schulz.⁷ From Eq. (13), when all χ '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,⁴ the shift of the Fermi energy from the VHS is a relevant parameter in driving this SDW $\rightarrow d$ -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 $La_{2-r}Ba_rCuO_4$ and $La_{2-x-y}Nd_ySr_xCuO_4$, near x = 1/8, where the striped phase is commensurately pinned, leading to long-ranged magnetic and charge order.¹⁹ 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 coterminus 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.¹² 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 ground state involving the V 6-vector.¹³

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