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Microscopic Electron Models with Exact SO(5) Symmetry

Silvio Rabello,1 Hiroshi Kohno,2 Eugene Demler,1 and Shou-Cheng Zhang1
1Department of Physics, Stanford University, Stanford, California 94305
2Department of Physics, University of Tokyo, Bunkyo-ku, Tokyo 113, Japan
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We construct a class of microscopic electron models with exact SO(5) symmetry between antiferromagnetic and d-wave superconducting ground states. There is an exact one-to-one correspondence between both single-particle and collective excitations in both phases. SO(5) symmetry breaking terms can be introduced and classified according to irreducible representation of the exact SO(5) algebra. The resulting phase diagram and collective modes are identical to that of the SO(5) nonlinear σ model. [S0031-9007(98)05903-1]

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One of the most interesting features of the high-\(T_c\) superconductivity is the close proximity and the interplay between the antiferromagnetic (AF) and the d-wave superconducting (dSC) phases. Recently, a theoretical formalism was introduced based on the concept of a SO(5) symmetry between these two phases, and the resulting field-theoretical model describes the cuprate phase diagram and collective modes in a unified framework [1]. It was argued that the microscopic Hubbard model supports an approximate SO(5) symmetry [1–3].

In this paper, we construct a class of microscopic electron models with exact SO(5) symmetry. In this model, degeneracy between the AF and dSC phases can be demonstrated exactly, and both the fermionic single-particle and the bosonic collective modes can be mapped onto each other with a precise one-to-one correspondence. This model can be used as a starting point around which SO(5) symmetry can be realized exactly by explicit microscopic Hamiltonians. The microscopic information extracted from this class of models, especially the behavior of the fermionic excitations across the AF/dSC transition, would greatly complement the effective field theory approach. Within this class of models, we have a consistent microscopic theory of the AF/dSC transition. Since both the AF and the dSC states are stable infrared fixed points, it is plausible that one can deform the parameters so that the microscopic SO(5) models can also serve as a paradigm for a much more general class of AF/dSC transitions, including those occurring in the high-\(T_c\) cuprates and 2D organics.

The first independent attempt to construct microscopic SO(5) invariant models was undertaken by Henley [5]. He independently made a crucial observation that, if one replaces the standard d-wave factor \(\cos p_x - \cos p_y\) by \(\text{sgn}(\cos p_x - \cos p_y)\), the SO(5) algebra introduced in [1] closes exactly.

It is easy to write down many electron models with exact SU(2) spin rotation invariance, because the electron operator \(c_{\mathbf{p} \sigma}\) forms a natural spinor representation of the SU(2) algebra. In writing down SU(2) invariant models, all we have to do is to contract the spinor indices in a natural way. Therefore, the first step towards constructing a SO(5) invariant electron model is to find a natural definition of a SO(5) spinor. Spinor representations of the SO(5) Lie algebra can be easily constructed using the Clifford algebra of five \(4 \times 4\) Dirac matrices [6] satisfying \[\{\Gamma^a, \Gamma^b\} = 2\delta_{ab}\ (a, b = 1, \ldots, 5),\] and the ten SO(5) rotation generators are given by \(\Gamma^{ab} = -i[\Gamma^a, \Gamma^b]\). In this paper we shall use the following explicit representation for the Clifford algebra:

\[
\Gamma^1 = \begin{pmatrix}
0 & -i\sigma_y \\
-i\sigma_y & 0
\end{pmatrix}, \\
\Gamma^2 = \begin{pmatrix}
0 & i\sigma_z \\
-i\sigma_z & 0
\end{pmatrix}, \\
\Gamma^3 = \begin{pmatrix}
\sigma_x & \sigma_y \\
-\sigma_y & -\sigma_x
\end{pmatrix}, \\
\Gamma^4 = \begin{pmatrix}
0 & -i\sigma_z \\
-i\sigma_z & 0
\end{pmatrix}, \\
\Gamma^5 = \begin{pmatrix}
\sigma_x & \sigma_y \\
-\sigma_y & -\sigma_x
\end{pmatrix},
\]

where \(\sigma = (\sigma_x, \sigma_y, \sigma_z)\) are the usual \(2 \times 2\) Pauli matrices, and the superscript \(t\) means transportation. We define a four-component spinor by

\[
\Psi_p = \{c_{p\uparrow}, c_{p\downarrow}, \phi_\pi(p) c_{p\uparrow}^\dagger + Q \phi_\pi(p) c_{p\downarrow}^\dagger, \phi_\pi(p) c_{p\downarrow}^\dagger + Q \phi_\pi(p) c_{p\uparrow}^\dagger\},
\]

where \(\phi_\pi(p) = \text{sgn}(\cos p_x - \cos p_y) = \pm 1\), and \(Q = (\pi, \pi)\). Since we have two spin degrees of freedom at a given momentum \(p\), such a description must be redundant. Indeed, one can easily see that the spinors with momenta outside the magnetic Brillouin zone are related to the spinors inside the magnetic Brillouin zone by an “\(R\) conjugation”

\[
\Psi_{p+Q} = \phi_\pi(p) R \Psi^*_{-p}.
\]

The \(R\) matrix is an invariant tensor of the SO(5) algebra enjoying the following properties: \(R \Gamma^a R = -\Gamma^a, R \Gamma^{ab} = \Gamma^{ab}\). In our representation it takes the form \(R = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\). [The existence of such a matrix is related
to the fact that the spinor representation of the SO(5) Lie algebra is pseudoreal. The $\sigma_\gamma$ matrix plays a similar role for SO(3). The $\Psi_{p\alpha}$ spinors obey the anticommutation relations:

$$\{\Psi^\dagger_{p\alpha}, \Psi^{}_{p'\beta}\} = \delta_{\alpha\beta} \delta_{pp'},$$

(3)

$$\{\Psi^{}_{p\alpha}, \Psi^\dagger_{p'\beta}\} = -\phi_\pi(p) R_{\alpha\beta} \delta_{pp'} Q.$$

(4)

If we restrict both $p$ and $p'$ inside the magnetic Brillouin zone, the right-hand side of the second equation vanishes and the $\Psi_{p\alpha}$ spinors commute in the same way as the $c_{p\alpha}$ spinors. They can be used to construct the SO(5) vector order parameter and the SO(5) algebra appears to be overconstrained. The commutator algebra does not close, and generates a direct sum of a scalar, a vector, and an antisymmetric tensor, i.e., $\Psi^{}_{p\alpha}$ transforms as a proper SO(5) spinor. They can be used to construct the SO(5) vector order parameter and the spinor indices. Under the SO(5) rotations generated by the $L_{ab}$, $\Psi^{}_{p\alpha}$ transforms as a proper SO(5) spinor

$$[L_{ab}, \Psi_{p\alpha}] = -\frac{1}{4} (\Gamma_{ab})_{\alpha\beta} \Psi_{p\beta}$$

(6)

for all values of $p$. Using these spinors, exact SO(5) invariant Hamiltonians can be constructed simply by proper contraction of the spinor indices.

We start with the kinetic term, and write it as

$$H_{\text{kin}} = \sum_{p,\sigma} e_p c^\dagger_{p,\sigma} c_{p,\sigma} = \frac{1}{2} \sum_p e_p \Psi^\dagger_p \Psi_p.$$  

(7)

We see that the property $e_{p+Q} = -e_p$, valid for a nn tight binding model, is crucial for this construction to work. In order to construct four-fermion interactions, we first note that a SO(5) spinor bilinear can in general be decomposed into a direct sum of a scalar, a vector, and an antisymmetric tensor, i.e., $4 \times 4 = 1 + 5 + 10$. Therefore, general SO(5) invariant four-fermion interactions can be expressed as

$$H_{\text{int}} = \sum_{p, p', q} V_1(p, p'; q) (\Psi^\dagger_p \Gamma^a \Psi_{p+q}) (\Psi^\dagger_{p'} \Gamma^a \Psi_{p'-q})$$

$$+ \sum_{p, p', q} V_2(p, p'; q) (\Psi^\dagger_p \Gamma^{ab} \Psi_{p+q}) (\Psi^\dagger_{p'} \Gamma^{ab} \Psi_{p'-q})$$

$$+ \sum_{p, q} V_0(p, p'; q) (\Psi^\dagger_p \Psi_{p+q}) (\Psi^\dagger_{p'} \Psi_{p'-q}).$$

(8)

Since $L_{ab}(p, q) = \Psi^\dagger_p \Gamma^{ab} \Psi_{p+q}$, $n_{a}(p, q) = \Psi^\dagger_p \Gamma^a \Psi_{p+q}$ and $\rho(p, q) = \Psi^\dagger_p \Psi_{p+q}$ are the true SO(5) tensor, vector, and scalar, respectively, for any $p$ and $q$; their inner products naturally gives a manifest SO(5) invariant Hamiltonian.

Among the terms in $H_{\text{int}}$, we concentrate on the vector interaction (first term) in all subsequent analysis, and assume a factorizable form $V_1(p, p'; q) = -V_1(q) w_p w_{p'}$. This form is not necessary, but simplifies calculations. In real space,

$$H_{\text{int},1} = -4 \sum_{\ell,n} V_1(R_{\ell} - R_n) e^{iQ \cdot (R_{\ell} - R_n)}$$

$$\times \left[ m_\ell \cdot m_n + \frac{1}{2} (\Delta_\ell \Delta^\dagger_\ell + \Delta^\dagger_\ell \Delta_\ell) \right].$$

(9)

Here, $m_\ell$ and $\Delta_\ell$ are Néel and d-wave pairing order parameters (operators) at site $\ell = R_\ell$, but with extended internal structures determined by $w_p$. For the simplest choice $w_p = 1$, they become

$$m_\ell = \frac{1}{2} (\psi_\ell \sigma \psi_\ell - \chi_\ell (\sigma \chi_\ell)) e^{iQ \cdot R_\ell},$$

(10)

$$\Delta^\dagger_\ell = \sum_j \phi_\pi(R_\ell - R_j) (c_{\ell j}^\dagger c_{\ell j} - c_{\ell j}^\dagger c_{\ell j}^\dagger).$$

(11)

Here, we introduced two-component spinors $\psi_\ell = (c_{\ell 1}, c_{\ell 2})$ and $\chi_\ell = (-e^{iQ \cdot R_\ell}) \times (b_{\ell 1}, b_{\ell 2})$ with $b_{\ell i} = \sum_j \phi_\pi(R_\ell - R_j) c_{\ell j}$. The pair wave function for dSC condensate is described by $\phi_\pi$ and is long ranged. For the choice $w_p = |\cos p_x - \cos p_y|$, we obtain

$$m_\ell = e^{iQ \cdot R_\ell}$$

$$2 \sum_i \phi_M(R_\ell - R_i) (\psi_\ell \sigma \psi_\ell - \chi_\ell \sigma \chi_\ell),$$

(12)

$$\Delta^\dagger_\ell = \sum_i \phi_M(R_\ell - R_i) (c_{i j}^\dagger c_{i j} - c_{i j}^\dagger c_{i j}^\dagger),$$

(13)

where

$$\phi_M(m,n) = \frac{4}{\pi^2} \frac{1 + (-)^{m+n}}{(m+n)^2 - 1}.$$  

(14)

The interaction between the centers of mass of $m$ or $\Delta$ fields is controlled by $V_1(R)$. If we take $V_1(q)$ to be a $\delta$ function at $q = Q$, the $\Delta$ part in $H_{\text{int},1}$ becomes the usual BCS reduced Hamiltonian for nn d-wave pairing. If
$V_1(q)$ is taken to be a Lorenzian around $q = Q$, the real space form of the spin interaction resembles the potential induced by the AF paramagnon exchange [7–9]. It is not difficult to find degeneracy between AF and dSC states in the usual treatment of mean field theories. However, their excitation spectra are generally different, and quantum fluctuations may remove this degeneracy. In the SO(5) invariant models, symmetry not only ensures exact degeneracy of the ground states, but also ensures exact one-to-one correspondence between their excitation spectra. This fact is formulated as follows:

**Theorem 1.** — If $|\Psi_0\rangle$ is a ground state of a SO(5) invariant Hamiltonian with AF broken symmetry (say, in the $n_2$ direction), i.e., $\langle \Psi_0 \mid n_{\alpha} \mid \Psi_0 \rangle = \delta_{2\alpha} A$, then $|\Psi'_0\rangle = e^{i(\pi/2)L_{12}} |\Psi_0\rangle$ is a degenerate ground state with dSC broken symmetry (in $n_1$ direction), i.e., $\langle \Psi'_0 \mid n_{\alpha} \mid \Psi'_0 \rangle = \delta_{1\alpha} A$. Furthermore, all excited states of the AF ground state can be mapped to excited states of the dSC ground state at the same energy by the $e^{i(\pi/2)L_{12}}$ operator.

The proof of this theorem is elementary, since $L_{12}$ commutes with the Hamiltonian, and $e^{-i(\pi/2)L_{12}} e^{i(\pi/2)L_{12}} = 1_2$. In the following, we shall illustrate this powerful theorem in an explicit mean field calculation. We take a “generalized BCS reduced Hamiltonian” by selecting $V_1(q) = V_1 \delta_{q0}$ in the vector interaction. The Green’s function in the presence of a mean field $\langle n_{p}^{a} \rangle = \frac{1}{4} \langle \Psi_{p}^{\dagger} \Gamma_{a} \Psi_{p} + Q \rangle$ is given by

$$G_{\alpha\beta}(p, p'; \omega) = -i \int dte^{it\omega} \langle T \Psi_{p,a}(t) \Psi_{p',\beta}(0) \rangle = \frac{(\omega + \epsilon_{p}) \delta_{\alpha\beta} \delta_{p,p'} + \Delta_{p}^{\alpha} \Gamma_{a\beta} \delta_{p,p'+Q}}{\omega^2 - \epsilon_{p}^2 - (\Delta_{p}^{\alpha})^2 + i\delta},$$

where $\Delta_{p}^{\alpha} = -16V_1 \omega_{p} \sum_{k} \omega_{k} \langle n_{k}^{\alpha} \rangle$. This manifestly SO(5) invariant Green’s function shows explicitly that the AF quasiparticles can be mapped onto dSC quasiparticles. In particular, the AF Green’s function (in the $n_2$ direction) can be obtained directly from the dSC Green’s function (in the $n_1$ direction) by a simple rotation: $G_{AF} = e^{-(\pi/2)L_{12}} G_{SC} e^{i(\pi/2)L_{12}}$. If we take $\omega_{p} = 1$, the AF quasiparticles have a full $s$-wave gap, while the dSC quasiparticles have a full $d$-wave gap, with step discontinuity at $\pm \pi/2, \pm \pi/2$ points. For the choice of $\omega_{p} = |\cos p_{x} - \cos p_{y}|$, the dSC quasiparticles have the usual cosine $s$-wave gap behavior, while the AF quasiparticles have an anisotropic s-wave gap with nodes at $\pm \pi/2, \pm \pi/2$ points (Fig. 1). Because the AF nodes are not “topological,” any small interactions will remove it [10]. In either case, the amplitude of the gaps is the same in both phases.

As symmetry-breaking perturbations to the above SO(5) invariant Hamiltonian, we consider two typical terms. One is the coupling to external fields $B_{ab}$, $H_{ext} = - \sum_{a < b} B_{ab} L_{ab}$. A particular example of this field is the chemical potential $\mu$.
of the Cartan (maximal commutative) subalgebra. In addition, we have the Casimir operator \( C = \sum_{a < b} L_{ab}^2 \), which commutes with all of the generators and has an eigenvalue \( l(l + 3) \). The set \( (Q, S_z, C) \) forms a Cartesian coordinate system labeling the quantum numbers of all states in the Hilbert space. If we consider only states with even number of electrons, these states form a pyramid, states in the Hilbert space. If we consider only states with changing the wave function of these states. In a system

\[ \sum_{a < b} L_{ab}^2 \]

as functions of \( \mu \) and \( v \). To diagonalize the Hamiltonian at half-filling, we employed the equations of motion (EOM) [4] and commutes with the Casimir operator, and simply shifting the energy of the \( Q \neq 0 \) states linearly without changing the wave function of these states. In a system with spontaneous symmetry breaking, lowest states with different \( l \) quantum numbers are separated by an inverse system size. In the infinite system limit, these shifts, due to chemical potential, converge to the parabola as depicted in Fig. 2 [11].

The symmetry-breaking terms, \( H_g \) and \( H_\mu \), produce the mass gap in the Goldstone mode spectrum. For \( H_g = 0 \), the mass of the \( \pi \) triplet mode is exactly \( 2|\mu| \). For finite \( H_g \) we employed the equations of motion (EOM) [12,13] for \( n^a \) to get the spectrum of collective modes. In the dSC state, we take \( (n_1, Q) = (n_1) \delta_{\mu, Q} \), and linearize the EOM to obtain the energy of the \( \pi \) triplet \( \omega_0 = 2\sqrt{\mu^2 - \mu_c^2} \), where \( \mu_c = (n_1) \sqrt{Q V_1} \), \( g = g(Q) \), and \( V_1 = V_1(Q) \), which is also consistent with the result of [1]. Similar calculation in the AF state gives the energies of the \( \pi \) doublet \( \omega_0 = 2(n_1) \sqrt{Q V_1 + g} \pm 2\mu \), where we assumed AF ordering along \( n_4 \). We therefore see that the two symmetry-breaking terms \( g \) and \( \mu \) partially compensate each other for the \( \pi \) triplet and \( Q = -2 \pi \) doublet.

In conclusion, we have constructed a class of electron models with exact SO(5) symmetry. If the model has an AF ground state at half-filling, it will have a dSC ground state away from half-filling. The phase diagram and the collective mode spectrum of these models are similar to the real high-\( T_c \) materials. However, our results also show that a significant SO(5) symmetry-breaking term \( H_g \) is required to produce the asymmetry in the size and angular distribution of the insulating and superconducting gaps. It is encouraging that this symmetry-breaking term transforms as a simple irreducible tensor under SO(5), and its consequences can be worked out systematically by the Wigner-Eckart theorem. Recent numerical calculations by Eder, Hanke, and Zhang [14] show that the two symmetry-breaking terms, \( H_g \) and \( H_\mu \), have compensating effects, so that a approximate SO(5) multiplet structure can be observed in the hole part of the spectrum in the \( t-J \) model.

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[6] Alternatively, one can also work out the spinor representation from Sp(4), the universal coupling group of SO(5).