

Interrelation of Superconducting and Antiferromagnetic Gaps in High- T_c Compounds: A Test Case for the SO(5) Theory

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Recent angle resolved photoemission data, which found evidence for a d -wave-like modulation of the antiferromagnetic gap, suggest an intimate interrelation between the antiferromagnetic insulator and the superconductor with its d -wave gap. It is shown here that a projected SO(5) theory, which explicitly takes the Mott-Hubbard gap into account, correctly describes the observed gap characteristics. Specifically, it accounts for the order of magnitude difference between the antiferromagnetic gap modulation and the superconducting gap and is also consistent with the gap dispersion.

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Angular-resolved photoemission spectroscopy (ARPES) recently provided evidence that points to a direct correlation between the d -wave symmetry of the superconducting (SC) gap and an observed d -wave-like modulation of the antiferromagnetic (AF) gap [1]. The “gap” structure in the AF phase, as found by the ARPES experiments in insulating $\text{Ca}_2\text{CuO}_2\text{Cl}_2$, is summarized in Fig. 1. These data display a d -wave-like dispersion in the one-electron spectral function $A(\vec{k}, \omega)$ with respect to the lowest energy state at $(\frac{\pi}{2}, \frac{\pi}{2})$, as revealed in the inset of this figure. This also becomes obvious when the energy difference $E(\vec{k}) - E(\frac{\pi}{2}, \frac{\pi}{2})$ is plotted versus the simple nearest-neighbor (nn) d -wave dispersion $|\cos k_x - \cos k_y|$. This “ $|d|$ -wave”-like gap [2] is a modulation of the uniform (s -wave) Mott-Hubbard gap of the order of $U \sim \text{eV}$ in the insulating state. The crucial point is that these photoemission data suggest that the $|d|$ component of the AF gap in the insulator is also the underlying reason for the celebrated pseudogap in the underdoped regime: this “high-energy” pseudogap of the order of the magnetic exchange $J \sim 0.2 \text{ eV}$ continuously evolves out of the insulating feature, as documented not only by the same energy scale but again by the same d -wave dispersion [3]. Since, on the other hand, this high-energy feature is closely correlated to the SC gap as a function of both doping and momentum [3–5], we finally arrive at a constraint on the microscopic theory: such a theory should be able to explain the interrelation between the SC gap and the AF gap modulation.

In this Letter, it is shown that a modified version of the SO(5) theory of high- T_c superconductivity, i.e., the *projected* SO(5) theory, provides rather naturally such an interrelation. This theory aims at unifying AF and SC via a symmetry principle, while at the same time explicitly taking the Mott-Hubbard gap into account. The projection is the crucial new ingredient, since the exact SO(5) symmetry requires charge excitations at half-filling to have the same gap as the collective spin-wave excitations [6–8]. This

condition is violated in a Mott-Hubbard insulator, which has a large gap ($\sim \text{eV}$) to all charge excitations while the spin excitations display no gap. In particular, in an exactly SO(5) symmetric description [7,8], the SC gap with its nodes would directly be mapped onto an AF gap, which then would have precisely the same magnitude and would vanish at the nodes $(\pm \frac{\pi}{2}, \pm \frac{\pi}{2})$. Taking the Mott-Hubbard gap into account amounts to properly projecting out the high-energy charge processes of order $\sim \text{eV}$ (Gutzwiller constraint) from the “low-energy” SO(5) rotation between AF and SC states [9].

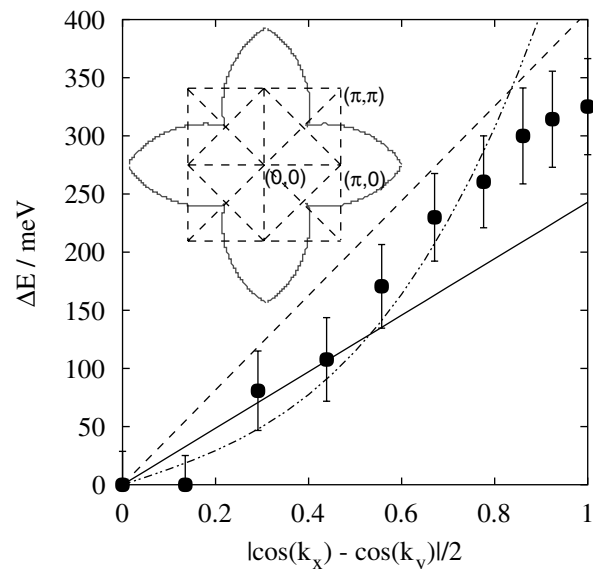


FIG. 1. ARPES results for $\text{Ca}_2\text{CuO}_2\text{Cl}_2$: $\Delta E = E(k) - E(\frac{\pi}{2}, \frac{\pi}{2})$ is plotted (dots with error bars) along the magnetic zone boundary against the nn d -wave function. The straight lines show the results of the SDW (solid line) and slave-boson (dashed) calculation based on a nn d -wave dispersion $d_{\vec{k}} = \cos k_x - \cos k_y$ for the SC gap (see text). The curved dash-dotted line gives the SB result using the extended d -wave function obtained from the fit of the Bi2212 SC gap in Fig. 2.

Our two main results are the following: (i) The projected SO(5) symmetry naturally introduces the s component of the AF gap associated with the large on-site Coulomb energy, which is absent in the case of pure SO(5) symmetry, and quantitatively relates the remaining $|d|$ component of the AF gap with the d -wave SC gap: In accordance with experiment, the d -wave SC gap is found to be of the order of $J/10$, whereas the obtained AF gap modulation is of the order of J . This is a direct consequence of the projection. (ii) The projected SO(5) theory accounts also for the dispersion of the two gap structures. It can also include deviations from the simple $\cos k_x - \cos k_y$ form, which have been recently reported both for SC [10] and AF [11] gaps.

Besides finding a modulation of the gap in the AF insulator, the recent ARPES experiment [1] also found a remnant Fermi surface of the AF insulator. This shows that it is appropriate to think of the AF insulator in terms of a condensate of *magnons* on top of a Fermi-liquid-like state, just like a superconductor can be viewed as a condensate of *Cooper pairs* on top of a Fermi-liquid state. To be more specific, the variational wave function of an AF insulator with Néel vector pointing in α direction is given by

$$|\Psi_{AF}\rangle \sim \prod_k (u_k + v_k c_{k+Q}^\dagger \sigma_\alpha c_k) |\Omega\rangle, \quad (1)$$

where c_k^\dagger is the spinor creation operator with wave vector k , $Q = (\pi, \pi)$ is the AF vector, σ_α are the Pauli spin matrices, u_k and v_k are the variational parameters, and $|\Omega\rangle$ is a half-filled Fermi-liquid-like state. A magnon is defined by the triplet operator $N_\alpha(k) = c_{k+Q}^\dagger \sigma_\alpha c_k$. On the other hand, a SC state is described by a formally completely equivalent state, where u_k and v_k are now the usual variational parameters, and the Cooper pair operator $B(k) = c_k \sigma_y c_{-k}$ replaces the magnon operator $N_\alpha(k)$ in Eq. (1). This “replacement” is exactly provided by the SO(5) rotation operator

$$\pi_\alpha = \sum_k g_k c_{k+Q} \sigma_\alpha \sigma_y c_{-k}, \quad (2)$$

where the form factor g_k can be written as $g_k = \text{sgn}(d_k^-)$. Here, d_k^- is the dispersion of the d -wave SC gap and for nn pairing would be given by the simple $\cos k_x - \cos k_y$ form. Recent experiments by Mesot *et al.* [10] indicate a deviation from this simple nn expression. This can be taken into account by choosing $d_k^- = b(\cos k_x - \cos k_y) + (1-b)(\cos 3k_x - \cos 3k_y)$ [12]. The parameter b (for $b \neq 1$) emphasizes the importance of longer-ranged (3rd nn) pairings [13].

The π operator rotates the magnon and Cooper pair operators into each other according to the following equation:

$$[\pi_\alpha, N_\beta(k)] = \delta_{\alpha\beta} g_k B(k), \quad [\pi_\alpha^\dagger, B(k)] = g_k N_\alpha(k). \quad (3)$$

From the above equation we see that, within an SO(5) symmetric description, a d -wave form of the Cooper pair

wave function will translate quite generally into a $|d|$ -form of the magnon wave function.

We now want to explore more quantitatively the consequences of assuming such a projected SO(5) symmetry for the high- T_c cuprates. Our starting point is the SC state. We first choose the simplest fermionic lattice Hamiltonian that reproduces the d -wave SC state of the high- T_c materials in a simple BCS mean-field description. We then perform an SO(5) rotation on the operator level that introduces the magnetic part of the interaction. The resulting SO(5)-invariant Hamiltonian takes thus the form

$$H_{\text{kin}} + H_{\text{int}} = \sum_{p,\sigma} \varepsilon_p c_{p,\sigma}^\dagger c_{p,\sigma} + \frac{V}{N} \times \sum_{\vec{r}_1, \vec{r}_2} \left\{ -\vec{m}(\vec{r}_1) \cdot \vec{m}(\vec{r}_2) + \frac{1}{2} [\Delta(\vec{r}_1) \Delta^\dagger(\vec{r}_2) + \Delta^\dagger(\vec{r}_1) \Delta(\vec{r}_2)] \right\}. \quad (4)$$

Here, H_{kin} stands for the kinetic energy part with band dispersion $\varepsilon_p = -2t(\cos p_x + \cos p_y)$, valid for a nearest-neighbor tight-binding model with hopping amplitude t . H_{int} contains a spin-spin interaction and a pair-hopping term [7,8]. The SC part of H_{int} is of reduced BCS form and is given in momentum space by $2V\{\Delta\Delta^\dagger + \Delta^\dagger\Delta\}$, where Δ is the usual d -wave order parameter $\Delta = \sum_p \frac{1}{2} d_{\vec{p}} c_{\vec{p},\uparrow} c_{-\vec{p},\downarrow}$. This BCS form in Δ and Δ^\dagger fixes the general SO(5)-invariant interaction with the coupling $V(\vec{p}, \vec{p}'; \vec{q})$ to be separable in momentum space and given by $V(\vec{p}, \vec{p}'; \vec{q}) = V \delta_{\vec{q}, \vec{Q}} |d_{\vec{p}}^-| |d_{\vec{p}'}^-|$. On the other hand, the Néel order parameter $\vec{m}(\vec{r})$ has an extended internal structure [14]. This internal structure is required by the SO(5) symmetry, and may, at least in principle, be tested in experiments. In particular, on a mean-field level, it may be related effectively to spatially extended hoppings t' and t'' [14], which have previously been introduced as parameters in t - J and Hubbard models to account for the AF gap anisotropy [15–17].

The Gutzwiller projection, which reduces the full SO(5) symmetry to a *projected* SO(5) symmetry, can be implemented by the introduction of a Hubbard U interaction and by taking the limit of large U . Therefore, we arrive at the following Hamiltonian:

$$H = (H_{\text{kin}} + H_{\text{int}}) + H_U + H_\mu, \quad (5)$$

where $H_U = U \sum_i n_{i\uparrow} n_{i\downarrow}$ is the standard Hubbard interaction in real space ($n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$) and $H_\mu = -\mu \sum_{i,\sigma} n_{i\sigma}$ denotes the chemical potential term.

The Hamiltonian (5) is further motivated by recent numerical and analytical results on much-used Hamiltonians [18–20], in particular the t - J and Hubbard model. These results have shown the presence of an approximate SO(5) symmetry in the low-energy bosonic excitations. However, the t - J model cannot explain the $|d|$ AF gap modulation in the fermionic sector. It, therefore, misses

an important piece of physics our current model contains (unless one introduces *ad hoc* values for t' , t'' ; see discussion above). The logic of our approach is similar in spirit to the phenomenological “Landau approach” to strongly correlated systems; i.e., rather than starting from first principles we construct an effective model from simple symmetry principles, and check whether it reproduces the low-energy experiments.

There are various ways to study the Hamiltonian in Eq. (5). Its physical content becomes transparent already on the simplest, i.e., Hartree-Fock mean-field level. Earlier work by Schrieffer *et al.* on the Hubbard model [21] shows that such a simple mean-field calculation can capture the basic physics also in the strong-coupling limit. Consider first the spin-density-wave (SDW)-type of solution for the Néel state. Here, the gap function $\Delta(\vec{p})$ is connected to the SDW mean field (polarized in the z direction) by the standard relation

$$\langle c_{\vec{p}+\vec{Q}}^\dagger \sigma_z c_{\vec{p}} \rangle = \frac{\Delta(\vec{p})}{2E(\vec{p})}, \quad (6)$$

where, as usual, $E(\vec{p}) = [v^2(\vec{p}) + \Delta^2(\vec{p})]^{1/2}$. When introduced in Eq. (5) for the Hamiltonian, this mean-field order parameter results in the self-consistency condition determining the gap $\Delta(\vec{p})$,

$$\frac{1}{N} \sum_{\vec{p}'} V(\vec{p}, \vec{p}') \frac{\Delta(\vec{p}')}{2E(\vec{p}')} = \Delta(\vec{p}) \quad (7)$$

(N being the number of lattice sites). Taking the factorized form of the SO(5) interaction (4), and including the Hubbard- U term, we obtain

$$V(\vec{p}, \vec{p}') = U + V|d_{\vec{p}}||d_{\vec{p}'}|. \quad (8)$$

First, note that the factorized form of the interaction $V(\vec{p}, \vec{p}')$ introduces a separable form of the AF gap,

$$\Delta^{\text{AF}}(\vec{p}) = \Delta_U + \Delta_{\text{mod}}|d_{\vec{p}}|. \quad (9)$$

For large values of the Hubbard interaction, Δ_U is of the order of U . Equation (9) then establishes the gap modulation $\sim \Delta_{\text{mod}}|d_{\vec{p}}|$ on top of a uniform gap in the AF.

Second, in formal analogy, in the d -wave SC state, the same gap equation (7) holds. As discussed in Eq. (3), the $|d_{\vec{p}}|$ -form factor has to be replaced by $|d_{\vec{p}}|g_{\vec{p}} = d_{\vec{p}}$ and, therefore, the relevant interaction is $V(\vec{p}, \vec{p}') = Vd_{\vec{p}}d_{\vec{p}'}$ (the U term drops out) resulting in the gap function

$$\Delta^{\text{SC}}(\vec{p}) = \Delta_{\text{SC}} \cdot d_{\vec{p}}. \quad (10)$$

Thus, both the AF gap in Eq. (9) and the SC gap have the required form. Our strategy now is to fit quantitatively the SC experimental gap (Fig. 2), then perform the SO(5) rotation, and compare the so obtained AF gap features with the ARPES results in Fig. 1. The SC gap is fixed in accordance with new ARPES data [10], allowing also for longer-ranged (3rd nn) interactions, obtained by using $b \neq 1$ ($b = 0.81$) in the extended d -wave form $d_{\vec{k}}$. However, we expect the precise value of b to be model dependent

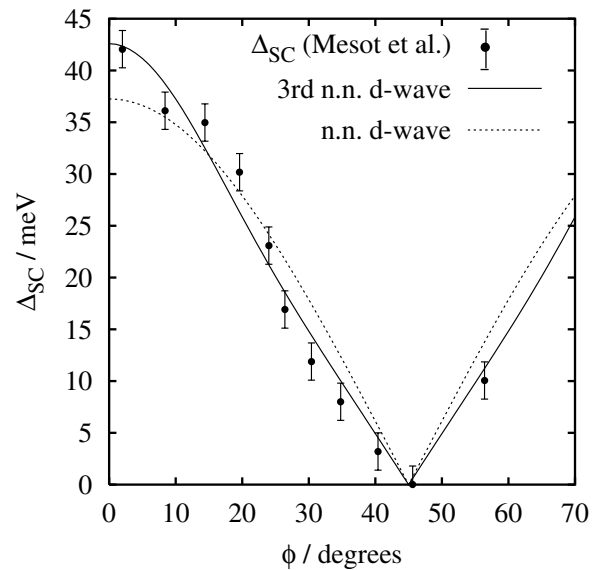


FIG. 2. ARPES results for the SC gap of Bi2212 in the underdoped region ($T_c = 75$ K) taken from Ref. [10] plotted against the Fermi angle ϕ (45 deg corresponds to $k_x = k_y$ and 0 deg to maximal k_x). The lines show fits to the data with both nn d -wave and 3rd nn d -wave functions [$d_{\vec{k}} = b(\cos k_x - \cos k_y) + (1 - b)(\cos 3k_x - \cos 3k_y)$]. With this fit procedure to the SC state, all free parameters in the theory are fixed (taking $t = 0.5$ eV as the energy scale).

and to differ for the two materials studied in Refs. [1] and [10]. The SO(5)-coupling strength V in Eq. (4) was chosen in such a way that [for both BCS and slave-boson (SB) evaluations, see below] it gives a d -wave gap of the correct order of magnitude in the SC phase, i.e., $\Delta_{\text{SC}} = 0.04t \approx J/10$ ($t = 0.5$ eV) [22].

Experiments tell us that while Δ_{SC} is of the order $J/10$, Δ_{mod} is an order of magnitude larger. To verify this independently from the above SDW/BCS evaluation, we have additionally used the slave-boson formalism, which we treat by the usual saddle-point approximation [23,24]. The essential observation, independent from the specific mean-field treatment, is then that, while the SO(5) interaction is responsible for the d -wave structure of both gaps, it is a different mechanism, namely the Hubbard gap, which is responsible for the experimentally observed order of magnitude differences in Δ_{SC} and Δ_{mod} .

This is clearly demonstrated in Fig. 3, which plots the amplitude Δ_{mod} of the AF d -wave-like modulation as a function of the Hubbard interaction U . We note that increasing U and, therefore, suppressing the doubly occupied states, strongly enhances the Δ_{mod} in both the SDW and SB evaluations. It is comforting to notice that the results are already converged at the commonly accepted value for $U = 8t$, i.e., the projection is almost complete here. Taking this value of U yields an AF gap modulation $\Delta_{\text{mod}} \approx 0.24t$ for SDW, and $\approx 0.41t$ for SB. Thus, we find a radically different energy scale between Δ_{mod} ($\sim J$) and Δ_{SC} ($\sim J/10$), in agreement with the ARPES data.

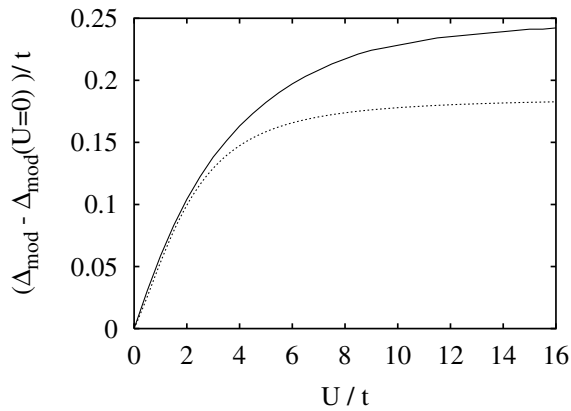


FIG. 3. The AF gap modulation $\Delta_{\text{mod}} - \Delta_{\text{mod}}(U=0)$ [25] obtained from the SDW (dotted line) and slave-boson (solid line) calculation as a function of the symmetry-breaking Hubbard interaction U . Note that the Δ_{mod} value for $U = 8t$ is already close to the saturated value obtained for complete projection ($U \rightarrow \infty$).

To summarize, our results on the d -wave dispersion, $d_{\vec{k}}$ in the SC gap and $|d_{\vec{k}}|$ in the AF gap modulation, are in general accordance with recent ARPES data [1,10]. Thus, the *projected* SO(5) rotation provides a definite link between the data points observed in two quite different phases, i.e., the insulating AF and the SC. This concept of projection is crucial, since, if one had used an exact SO(5) theory, without the physically relevant term H_U , one would have obtained an AF gap with nodes. Moreover, as demonstrated here, H_U is pivotal in explaining the order of magnitude differences between the SC gap Δ_{SC} and the d -wave-like modulation of the AF gap Δ_{mod} . Just like the neutron resonance mode can be interpreted as the reflection of AF correlation in the SC state [6,18], the ARPES experiment can be interpreted as the reflection of the SC correlation in the AF state.

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[13] Notice that this generalized form factor $g_{\vec{k}}$ satisfies the SO(5) group closure requirements in the same way as the $\text{sgn}(\cos k_x - \cos k_y)$ form introduced in Refs. [7,8]. Our form has the advantage of a more appropriate description of the experiments.

[14] The extended internal structure of $\vec{m}(\vec{r}_1)$ [i.e., $\vec{m}(\vec{r}_1) = \sum_{\vec{r}_2} \frac{1}{2} w(\vec{r}_1 - \vec{r}_2) e^{i\vec{Q}\vec{r}_2} c_{\vec{r}_1}^\dagger \vec{\sigma} c_{\vec{r}_2}$, where $\vec{\sigma}$ are the usual 2×2 Pauli matrices] introduces on a mean-field level [replacing $\vec{m}(\vec{r}_2)$ in Eq. (4) by twice its expectation value $\langle \vec{m}(\vec{r}_2) \rangle$] longer-ranged hopping terms t' (next nn) and t'' (third nn). Similar to the commonly used spatially extended hoppings [15–17], their signs alternate. This stems from the fact that $w(\vec{r})$ is the Fourier transform of $|d(\vec{p})|$ and, for nn d wave, takes the values [$\vec{r} = (m, n)$ on the 2D lattice]: $w(m, n) = 0$, if $m + n = \text{odd}$, $w(0, 0) = \frac{8}{\pi^2}$, $w(1, 1) = -\frac{8}{3\pi^2}$, and $w(2, 0) = \frac{8}{9\pi^2}$, etc. This results in $t' = \Delta_{\text{mod}} w(1, 1) \approx 0.07t$ and $t'' = \Delta_{\text{mod}} w(2, 0)$ with $t''/t' = -1/3$, where we used $\Delta_{\text{mod}} = 0.243t$ (the result of our nn SDW calculation).

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