

PROJECTED SO(5) HAMILTONIAN FOR CUPRATES AND ITS APPLICATIONS

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The projected SO(5) (pSO(5)) Hamiltonian incorporates the quantum spin and superconducting fluctuations of underdoped cuprates in terms of four bosons moving on a coarse grained lattice. A simple mean field approximation can explain some key features of the experimental phase diagram: (i) The Mott transition between antiferromagnet and superconductor, (ii) the increase of T_c and superfluid stiffness with hole concentration x and (iii) the increase of antiferromagnetic resonance energy as $\sqrt{x-x_c}$ in the superconducting phase. We apply this theory to explain the “two gaps” problem in underdoped cuprate SNS junctions. In particular we explain the sharp subgap Andreev peaks of the differential resistance, as signatures of the antiferromagnetic resonance (the magnon mass gap). A critical test of this theory is proposed. The tunneling charge, as measured by shot noise, should change by increments of $\Delta Q = 2e$ at the Andreev peaks, rather than by $\Delta Q = e$ as in conventional superconductors.

1. Introduction

The underdoped regime of high- T_c cuprate superconductors exhibits a pairing energy (called pseudogap Δ_p) which is much larger than the superconducting transition temperature T_c . Δ_p is measured by NMR,¹ tunneling,² photoemission³ and other probes, as a sharp decrease in the single particle density of states below Δ_p at temperatures below $2\Delta_p$. Assigning Δ_p to the local pairing energy, is consistent with the observed anisotropy of $|\Delta_p(\mathbf{k})|$ in momentum space³ as expected for a d -wave symmetry of the pair wavefunction.

In sharp contrast to conventional BCS superconductors, T_c and Δ_p are *not* proportional.⁴ While Δ_p decreases with hole doping x , T_c grows with x , as does the superfluid density ρ_s . The latter relation is not coincidental as argued by Emery and Kivelson.⁵ Basically, since ρ_s is small at low doping, superconductivity is destroyed by thermal phase fluctuations, and thus T_c is determined by the Kosterlitz–Thouless transition temperature $T_c \sim \rho_s$, and not by pair breaking effects which are suppressed at $T_c \ll 2\Delta_p$.

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The behavior of $\rho_s \sim x$ is even more unconventional. It demonstrates that the correct number of charge $2e$ bosons is proportional to the number of doped *hole pairs* away from the half-filled Mott phase. The Mott phase exhibits long range antiferromagnetic (AFM) correlations. This is a consequence of the strong local Hubbard interactions, which cannot be easily handled as a weak coupling perturbation of the electron gas.

The proximity of the AFM phase to the superconductor suggests that the effective Hamiltonian for the low energy collective modes would describe 4 bosons: three magnons of the Heisenberg antiferromagnet, and the hole pairs. In fact, in addition there are gapless fermionic particle-hole excitations near the nodes of $\Delta_p(\mathbf{k})$, $\mathbf{k} \approx (\pm\pi/2, \pm\pi/2)$.

In the AFM phase, one magnon branch condenses, yielding a finite staggered magnetization, while the other two become the two spin wave modes. At higher doping, in the superconducting phase, AFM order disappears which allows these modes to become massive with mass Δ_s , and for optimally doped YBCO they are observed by inelastic neutron scattering as a resonance at around 40 meV near the AFM wavevector.

Such a model was introduced⁶ as the “*projected SO(5) (pSO(5)) theory*”. This model is constructed by projecting out doubly occupied configurations from the local two-site SO(5) multiplets. The remaining states are local singlets, triplets and hole pairs, which define the local bosons.

In the following, we review the pSO(5) model and its primary consequences by mean field theory. The important predictions are $\rho_s \sim x$, and that $\Delta_s(x) \sim \sqrt{x - x_c}$.

We then use the pSO(5) model to predict current singularities in Superconductor-Normal-Superconductor (SNS) junctions,⁷ and propose a future experimental test of this theory. *The tunneling charges, as measured by shot noise, should change by $2e$ at the Andreev peaks, rather than by e as in conventional superconductors.*

2. The Model

The large onsite Hubbard repulsion between electrons is imposed by an *a priori* projection of doubly occupied states from the Hilbert space.⁹

The undoped vacuum $|V\rangle$ is a half-filled Mott insulator in a quantum spin liquid state. The pSO(5) vacuum possesses short range antiferromagnetic correlations. A translationally invariant realization of $|V\rangle$ on the microscopic square lattice, is the short range resonating valence bonds (RVB) state.^{10,11} Since local singlets without holes and double occupation can only be produced with even number of sites, we must choose a coarse grained lattice in order to define the vacuum and the Fock space.

If one defines a superlattice of dimers on the original square lattice, a Fock vacuum can be explicitly constructed in terms of electronic operators as dimer

singlets, where i labels a dimer.

$$|V\rangle_i = \frac{1}{\sqrt{2}} \left(c_{i1,\uparrow}^\dagger c_{i2,\downarrow}^\dagger - c_{i1,\downarrow}^\dagger c_{i2,\uparrow}^\dagger \right) |0\rangle_i, \tag{1}$$

where $|0\rangle_i$ is an empty state of electrons. The hole pairs are simply

$$b_{hi}^\dagger |V\rangle_i = |0\rangle_i. \tag{2}$$

The triplets are defined as bosonic excitations of the RVB vacuum i.e.

$$\begin{aligned} b_{zi}^\dagger |V\rangle_i &= \frac{1}{\sqrt{2}} \left(c_{i1,\uparrow}^\dagger c_{i2,\downarrow}^\dagger + c_{i1,\downarrow}^\dagger c_{i2,\uparrow}^\dagger \right) |0\rangle_i, \\ b_{xi}^\dagger |V\rangle_i &= \frac{1}{\sqrt{2}} \left(c_{i1,\uparrow}^\dagger c_{i2,\uparrow}^\dagger + c_{i1,\downarrow}^\dagger c_{i2,\downarrow}^\dagger \right) |0\rangle_i, \\ b_{yi}^\dagger |V\rangle_i &= \frac{1}{\sqrt{2}} \left(c_{i1,\uparrow}^\dagger c_{i2,\downarrow}^\dagger - c_{i1,\downarrow}^\dagger c_{i2,\uparrow}^\dagger \right) |0\rangle_i. \end{aligned} \tag{3}$$

Out of the undoped RVB vacuum $|V\rangle$, b_h^\dagger create charge $2e$ bosons (hole pairs) and b_α^\dagger , $\alpha = x, y, z$ create a triplet of antiferromagnetic, spin one magnons. For the square lattice, a similar construction which preserves the lattice rotation group and has explicit d -wave symmetry of the hole pairs bosons, will be presented in a forthcoming publication.⁸

The lattice pSO(5) Hamiltonian is

$$\begin{aligned} \mathcal{H}^{\text{pSO}(5)} &= \mathcal{H}^{\text{charge}} + \mathcal{H}^{\text{spin}} + \mathcal{H}^{\text{int}} + \mathcal{H}^{\text{Coul}} + \mathcal{H}^{\text{ferm}} \\ \mathcal{H}^{\text{charge}} &= (\epsilon_c - 2\mu) \sum_i b_{hi}^\dagger b_{hi} - \frac{J_c}{2} \sum_{\langle ij \rangle} \left(b_{hi}^\dagger b_{hi}^\dagger + \text{H.c.} \right), \\ \mathcal{H}^{\text{spin}} &= \epsilon_s \sum_{i\alpha} b_{\alpha i}^\dagger b_{\alpha i} - J_s \sum_{\alpha \langle ij \rangle} n_i^\alpha n_j^\alpha, \\ \mathcal{H}^{\text{int}} &= W \sum_i : \left(b_{hi}^\dagger b_{hi}^\dagger + \sum_\alpha b_{\alpha i}^\dagger b_{\alpha i}^\dagger \right)^2 :, \end{aligned} \tag{4}$$

where $:() :$ denotes normal ordering, and $n_i^\alpha = (b_{i\alpha}^\dagger + b_{i\alpha})/\sqrt{2}$ is the Néel spin field. \mathcal{H}^{int} describes short range interactions between bosons, and $\mathcal{H}^{\text{Coul}}$ describes the long range Coulomb interactions. $\mathcal{H}^{\text{ferm}}$ describes coupling to the nodal (fermionic) quasiparticles, which contribute a finite density of single electron states at low energies. We shall not compute the fermion contributions, and will discuss them in detail elsewhere.⁸

3. Mean Field Theory: Results

The uniform mean field approximation to Eq. (4) is straightforward.⁶ It amounts to replacing $b_{\gamma i} \rightarrow \langle b_\gamma \rangle$, $\gamma = h, \alpha$. The order parameters are related to experimental observables: the Bose condensate of hole pairs is the superconducting order

parameter

$$x = \langle b_h^\dagger \rangle = \left\langle \sum_{ij} d_{ij} c_{\uparrow i} c_{\downarrow j} \right\rangle, \tag{5}$$

where d_{ij} is the normalized short range pair wavefunction with d wave symmetry. Bose condensation of magnons yields the staggered magnetization

$$y = \langle b_z \rangle = \langle n^z \rangle. \tag{6}$$

The $T = 0$ variational energy of $\mathcal{H}^{\text{charge}} + \mathcal{H}^{\text{spin}} + \mathcal{H}^{\text{int}}$ is

$$\frac{E^{\text{MFT}}}{\mathcal{N}} = \left(\epsilon_c - 2\mu - \frac{z}{2} J_c \right) x^2 + \left(\epsilon_s - z J_s \right) y^2 + W(x^2 + y^2), \tag{7}$$

where $z = 4$ is the square lattice coordination and \mathcal{N} is the lattice size. Minimizing $E(x, y)$ we find a first order transition between two phases:

$$\begin{aligned} \mu < \mu_c & \quad \text{AFM insulator: } x = 0, y \neq 0 \\ \mu > \mu_c & \quad d\text{-SC: } x \neq 0, y = 0 \end{aligned}$$

where

$$\mu_c = \frac{1}{2} \left[(\epsilon_c - \epsilon_s) - \left(\frac{z}{2} J_c - z J_s \right) \right]. \tag{8}$$

At $\mu < \mu_c$ we have an undoped Mott insulator with no hole pair bosons, and where the magnons Bose-condense. The condensate supports a finite staggered magnetization

$$|\langle n^\alpha \rangle|^2 = \frac{1}{W} \left(2J_s - \frac{1}{2} \epsilon_s \right) \equiv m_s^2, \quad \mu < \mu_c. \tag{9}$$

Expanding the mean field Hamiltonian to second order in the Bose operators, one obtains two linear spin wave modes at

$$\omega = c|\mathbf{q}|, \quad c = \frac{2\sqrt{2}J_s}{\hbar}. \tag{10}$$

c is the semiclassical spinwave velocity which agrees with semiclassical limit of the Heisenberg antiferromagnet.

At $\mu > \mu_c$ the ground state becomes doped with hole pairs which Bose-condense into a superconducting phase with an order parameter

$$|\langle b_h^\dagger \rangle|^2 = \frac{(\mu - \mu_c)}{W} + m_s^2, \quad \mu > \mu_c. \tag{11}$$

The mean field phase stiffness is given by $\rho_c = J_c \langle b_i^\dagger \rangle^2$, and therefore Eq. (11) explains why ρ_c increases with chemical potential (and doping) in the underdoped superconducting regime, as observed experimentally.¹² Quantum phase fluctuations which increase with $\rho_c^{-1/2}$ significantly reduce the mean field order parameter (11) near the transition.

Long range interactions in $\mathcal{H}^{\text{Coul}}$, frustrate the first order transition and create intermediate (possibly incommensurate) phases,⁶ which we shall not discuss here.

Analysis of the linear quantum fluctuations about mean field theory in the superconducting phase, when $y = 0$, yields three massive magnons (of spin 1). Their mean field Greens function approximates the spin structure factor

$$S_{\alpha\alpha'}(\omega, \mathbf{q}) \approx s_0 \frac{\delta_{\alpha\alpha'}}{\omega^2 - c^2(\mathbf{q} - \vec{\pi})^2 - \Delta_s^2}. \quad (12)$$

Here c is the spin wave velocity, and s_0 is a normalization factor. The poles of Eq. (12) have a mass gap at Δ_s . The mean field magnon gap is found to depend on the chemical potential as follows:

$$\begin{aligned} \Delta_s &= 2\sqrt{(\mu - \mu_c)(\mu - \mu_c + 2J_s)} \propto \sqrt{x - x_c}, \\ c(\mu) &= 2\sqrt{2}J_s\sqrt{1 + \frac{\mu - \mu_c}{2J_s}}, \end{aligned} \quad (13)$$

which by Eq. (11) also implies that Δ_s^2 increases, and the magnon dispersion stiffens at higher doping.

Thus the pSO(5) mean field theory can explain the systematic increase of Δ_s with T_c which has been observed by Fong *et al.*¹³ The doping dependent resonance energy $\Delta_s(\delta)$ increases¹³ between $\Delta_s(0.5) = 25$ meV (with $T_c = 52$ K), and $\Delta_s(1) = 40$ meV (at $T_c = 92$ K).¹³

4. SNS Junction: KBT Theory

Peaks in the differential resistance of Superconducting–Normal–Superconducting (SNS) junctions have been customarily interpreted using the theory of multiple Andreev reflections, following Klapwijk, Blonder and Tinkham (KBT).¹⁴

KBT theory treats two conventional superconductors with a single s -wave BCS quasiparticle gap Δ , separated by a free electron metal. Electrons traversing the metal are Andreev reflected back as holes, gaining energy increments eV at each traversal (as depicted in Fig. 1). Peaks in the differential resistance appear at voltages $2\Delta/ne$, and are due to the $(E - \Delta)^{-1/2}$ singularity in the quasiparticles' density of states.

However, in cuprate SNS junctions, such as $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$ – $\text{YBa}_2\text{Cu}_{2.55}\text{Fe}_{0.45}\text{O}_y$ – $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$ examined by Neshet and Koren,¹⁵ application of KBT theory is problematic. A naive fit to KBT expression faces the two gaps puzzle, i.e. an “Andreev gap” is of order $\Delta \approx 16$ meV, while the tunneling gap is about three times larger,¹⁶ and scales differently with T_c . Without perfect alignment of the interfaces, it is hard to understand the observed sharpness of peaks¹⁵ since the d -wave gap is modulated at different directions. Moreover, the barrier is by no means a “normal” metal devoid of interactions: it is an underdoped cuprate with antiferromagnetic correlations and strong pairing interactions as evidenced by a large proximity effect.¹⁷

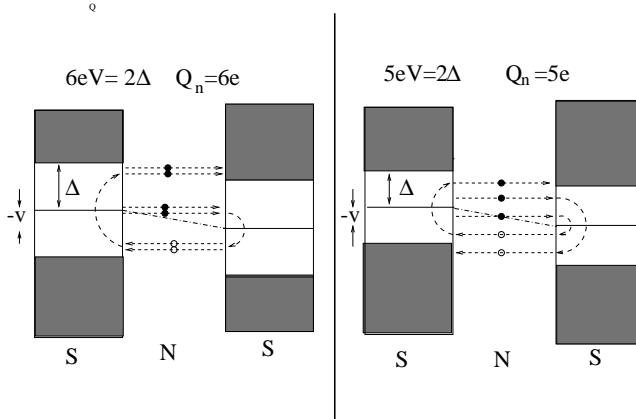


Fig. 1. **KBT Theory.** Differential resistance peaks of $n = 6$ (left diagram), and $n = 5$ (right diagram), involve a cascade of n Andreev reflected charges traversing the normal metal. Singular dissipation is due to emission of quasiparticles above the s -wave gap. Filled (empty) circles denote electrons (holes) in the normal barrier.

In the following sections we review an alternative explanation for the differential resistance peaks series,⁷ which takes into account the strong correlations in the pseudogap regime. Our analysis resolves Duetscher’s two energy scales puzzle.⁴

5. SNS Junctions: pSO(5) Theory

We consider a junction, where the barrier (N) has no superconducting or magnetic order $\langle b_h^\dagger \rangle = 0, \langle n^\alpha \rangle = 0$. We derive on general grounds the form of the effective tunneling Hamiltonian between superconductors as follows.

An integration of the barrier’s charged bosons b_h out of the path integral results in an effective action \mathcal{S}^{tun} which couples the charges of the two superconductors. $\mathcal{S}^{\text{tun}}[b_{hL}, b_{hR}, b_\alpha]$ explicitly depends on the hole pairs bosons on the left and right interfaces, and on the magnons in the barrier. By charge conservation, an expansion of \mathcal{S}^{tun} as a power series leaves only terms with equal number of b_h ’s and b_h^\dagger ’s. By spin conservation, the magnon terms are singlets and hence at least bilinear in n^α .

This expansion leads to a series of tunneling terms. For the Andreev peaks we retain only the leading order terms (in b^\dagger, b) which are

$$\begin{aligned} \mathcal{H}^{\text{tun-mag}} &= \sum \frac{\delta^{2n+2} \mathcal{S}}{\delta b_{hi_1} \dots \delta b_{hi_{2n}} \delta n^\alpha \delta n^\alpha} b_{hi_1} \dots b_{hi_{2n}} n^\alpha n^\alpha, \\ &= - \sum_n (\mathcal{A}_n^\dagger + \mathcal{A}_n^\dagger), \\ \mathcal{A}_n &= \sum_{y_1 \dots y_{2n}, \mathbf{x}, \mathbf{x}'} T_n b_{hL,1}^\dagger \dots b_{hL,n}^\dagger b_{hR,n+1}^\dagger \dots b_{hR,2n}^\dagger \sum_\alpha n^\alpha(\mathbf{x}) n^\alpha(\mathbf{x}'). \end{aligned} \quad (14)$$

\mathcal{A}_n^\dagger describes a simultaneous tunneling of n hole pairs from the left to the right

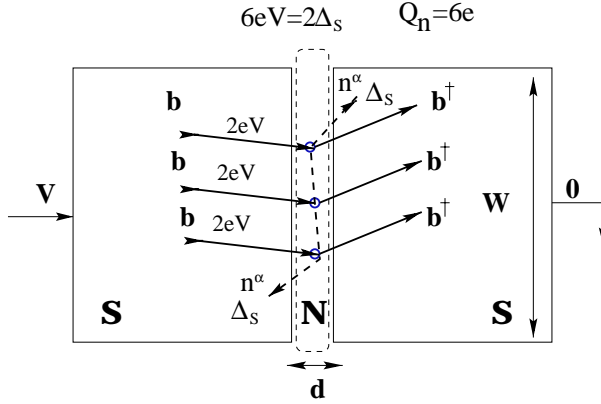


Fig. 2. **pSO(5) theory for Andreev peaks in cuprate SNS junctions.** Three hole pairs co-tunneling from left to right, generate a pair of magnons. At the antiferromagnetic resonance threshold $6eV = 2\Delta_S$, this process contributes to the $n = 3$ peak of the differential resistance. The diagram contains lowest order contributions of hole pairs-magnon interactions to the tunneling vertex T_3 .

superconductor, coupled to a magnon pair excitation. T_n is the tunneling vertex function, which depends on the bosons positions.

The energy transfer mechanism is depicted diagrammatically in Fig. 2. We do not compute T_n 's which depend on the details of the barrier and the interfaces. A “good” N barrier is defined to have sizeable T_n , if multiple pair tunneling terms are to be observed. This requires a thin barrier with slowly decaying spin and charge correlations.¹⁷ It is important to note that multiple pair tunneling, i.e. the differential resistance peaks at $n > 1$, depends on strong anharmonic interactions between the hole pairs and magnons. *These interactions are an essential part of the pSO(5) theory* as modelled by \mathcal{H}^{int} in Eq. (4).

The junction's conductance is calculated in the standard fashion¹⁸: the bias voltage V transforms the left bosons $b_{h_L} \rightarrow e^{i2eVt} b_{h_L}$, which yields time dependent operators $\mathcal{A}_n(t)$. The current is calculated by second order perturbation theory in $\mathcal{H}^{\text{tun-mag}}$ yielding

$$I = \sum_n 2ne X_n^{\text{ret}}(2eV), \quad (15)$$

$$X_n^{\text{ret}}(\omega) = i \int_0^\infty dt e^{i\omega t} \langle [A_n^\dagger(t), A_n^\dagger] \rangle.$$

For singular contributions I^{sing} , we ignore superconducting condensate fluctuations $b_h^\dagger - \langle b_h^\dagger \rangle$, which have a smooth spectrum. Similarly, we ignore the frequency dependence of $T_n(\omega)$. Setting $b_R^\dagger \rightarrow \langle b_h^\dagger \rangle$ and $b_L^\dagger \rightarrow e^{i2eVt} \langle b_h^\dagger \rangle$ leads to

$$I^{\text{sing}} = \sum_n 2ne \sum_{\substack{|q_x| \leq \pi/d \\ |q_y| \leq \pi/W}} \langle b_h^\dagger \rangle^{4n} |T_n[\mathbf{q}]|^2 \Im \sum_\omega S(\mathbf{q}, i\omega + 2neV + i0^+) S(-\mathbf{q}, i\omega), \quad (16)$$

where the barrier dimensions are $d \times W$ (see Fig. 2), and \sum_ω is a Matsubara sum.

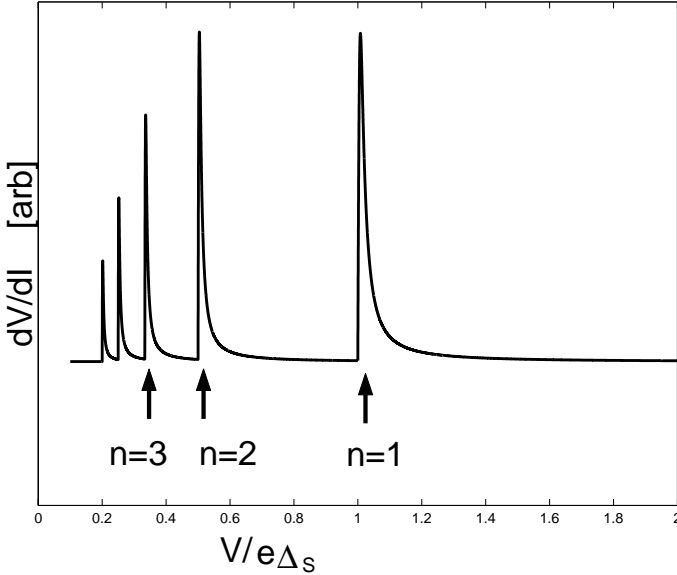


Fig. 3. **pSO(5) Andreev peaks.** Eq. (17) is plotted for a choice of $t_n/\Delta_s^{3/2} = 2^{-n}10^{-4}$, $n \leq 5$, and a background conductance of unity. Below the n th peak, the excess tunneling charge is $2ne$, rather than BTK’s ne .

For a nearly antiferromagnetic “N” barrier, $T_n(\mathbf{x} - \mathbf{x}')$ in (14) decays slowly with the distance between magnons. Thus for a narrow barrier $d \ll W$, the magnons are excited at $q_y \approx 0$, and the momentum sum reduces to a one-dimensional sum over q_x . At zero temperature we obtain

$$\begin{aligned}
 I^{\text{sing}} &= \sum_n 2ne \langle b_h^\dagger \rangle^{4n} |T_n[0]|^2 s_0^2 \int \frac{dq_x}{2\pi} \frac{\delta(2neV - 2\sqrt{c^2q_x^2 + \Delta_s^2})}{2(\Delta_s^2 + c^2q_x^2)} \\
 &\approx \sum_n t_n \frac{\theta(neV - \Delta_s)}{\Delta_s^{3/2} \sqrt{neV - \Delta_s}}.
 \end{aligned}
 \tag{17}$$

The last expression emphasizes the singular form of $I^{\text{sing}}(V, \Delta_s)$ at the peaks. For a large background conductance $dI/dV \gg dI^{\text{sing}}/dV$, the inverse square root singularities in I^{sing} create peaks in the differential resistance dV/dI at voltages

$$V_n = \frac{\Delta_s}{ne}, \quad n = 1, 2, \dots, \quad Q_n = 2ne,
 \tag{18}$$

where Q_n is the excess tunneling charge below the n th peak. Note that Q_n changes in increments of $2e$. The differential resistance peak series is depicted in Fig. 3, for weak broadening of the singularities and an arbitrary set of coefficients t_n .

6. Discussion, and Proposed Experiment

We have seen that magnon pair creation induces peaks in the differential resistance which are similar *in appearance* to the Andreev peaks of the KBT mechanism.

The crucial difference is that here the singular dissipative process does *not* involve Cooper pair breaking, but low energy antiferromagnetic excitations. In the KBT mechanism, a single sharp gap-like feature can be obtained in a d wave superconductor only by precise alignment of the a - b axes of the two superconductors.

Here, one only requires the junction to be flat in the transverse direction, such that q_y is conserved and the charge pairs are coupled mostly to the one-dimensional singularity of the magnon density of states. This requirement is less stringent for weakly dispersive magnons near the resonance.

In KBT theory for two identical superconductors, the peaks appear at voltages $V_n^{\text{KBT}} = 2\Delta/(ne)$, $n = 1, 2, \dots$ which are the upper threshold for tunneling of charges $Q_n = ne$. Thus, KBT allows both even and odd number of electron charges to participate in the multiple Andreev reflection process, as depicted in Fig. 1, while the pSO(5) theory expects only pair charges $Q_n = 2ne$.

Observation of Andreev reflection enhanced shot noise $S(V)$ has been reported by Dieleman *et al.*¹⁹ in a conventional SNS junction. They have measured the tunneling charge via the relation²⁰ $S = 2Q_n I(V_n)$. The increment of charge at the first Andreev peak at 2Δ was clearly seen to be of magnitude e .

We propose that a similar measurement in YBCO junctions could provide a decisive discrimination between the processes of Figs. 1 and 2. The goal is to measure the charge *increments* $Q_n - Q_{n-1}$ at any peak position V_n , $n = 1, 2, \dots$ and see whether they are of magnitude $2e$ rather than e . The measurement would probably involve a careful subtraction of the large but smooth background quasiparticle contribution to the current and the noise spectrum. We eagerly look forward to results of such experiments.

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classical ground state manifold. The vacuum is a projected RVB state and not an empty Fermi surface. These are some of the crucial differences between the pSO(5) theory and the earlier unprojected SO(5) theory of S.-C. Zhang, *Science* **275**, 1089 (1997).

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