Tunneling spectroscopy of $s\pi$ pairing state as a model for FeAs superconductors

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We present the self-consistent Bogoliubov-de Gennes calculations of an $s\pi$ pairing state of two band superconductivity as a model for the FeAs superconductors. The $s\pi$ state is an $s$-wave pairing state with an internal $\pi$ phase, that is, nodeless gaps on each band but with the opposite sign. The novel features of this state are investigated by calculating the local density of states of the $\pi$ phase superconductor/normal metal bilayers. Because of the sign reversal between the two condensates, the zero bias conductance peak appears as observed in tunneling spectroscopy experiments on FeAs superconductors. This eliminates the major obstacle to establish the $s\pi$ state as the pairing symmetry of the FeAs superconductors.

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Introduction – The recent discovery of the iron based pnictides superconductors generated enormous interests in the community. Like the cuprate superconductors, the pnictides are highly two-dimensional, the undoped parent materials are in the antiferromagnetic state, and superconductivity emerges when the antiferromagnetism is suppressed upon doping either electrons or holes into the FeAs planes. The urgent question is the pairing mechanism of the FeAs superconductors. This will hopefully pave the way to coherently understand the still elusive pairing mechanism of the high temperature superconductivity. The first step towards this goal is to establish the pairing symmetry of the FeAs superconductors.

Conflicting experimental results are being reported with regard to the orbital pairing symmetry. Some experiments are unambiguously suggesting a fully gapped nodeless superconducting state, while others point towards a gap with nodes: The several independent ARPES experiments on single crystals reported the full gaps around the hole Fermi surface although the gap feature is less clear around the electron Fermi surface. The temperature dependence of the penetration depth strongly suggests a nodeless gap structure. The infrared spectroscopy observed the superconductivity induced features which were best described in terms of $s$-wave pairing.

The evidences for nodes are also accumulating: The nuclear spin-lattice relaxation rate $1/T_1$ clearly showed no coherence peak and $\sim T^3$ dependence below $T_c$, which are consistent with the $s$-wave pairing formulation. Other point contact and tunneling spectroscopy measurements also reported the ZBP which strongly suggests a sign change of the pairing order parameter.

Many ideas have been put forward to understand the seemingly conflicting experimental observations on the FeAs materials. Among them, particularly appealing is the sign changing $s$-wave pairing state as advanced by Mazin and coworkers. It seems to be able to explain the experimental observations indicating the full gap as well as a gap with nodes. It was noticed early on that there exists this type of solution to a multi-band BCS gap equation. It is quite exciting that it seems to be actually realized in the pnictides. We adapt this proposal in this Letter, and call it “$s\pi$” pairing state because of its natural connection with other $\pi$ states. It is interesting to note the similarity between the internal $\pi$ state of the $s\pi$ pairing and the “external” $\pi$ state of the superconductor/ferromagnet (S/F) bilayers. It is well established that a Cooper pair in the F side of an S/F bilayer picks up a non-zero center of mass momentum and the singlet pairing order parameter oscillates as a function of position in the F side. The superconductivity induced suppression of local density of states (LDOS) in the subgap energy range becomes enhanced where the order parameter changes its sign. Similarly, the internal $\pi$ state is expected to exhibit the zero...
bias conductance enhancement in the subgap region \[32\].

We will show that it is indeed the case. This eliminates the major obstacle to establishing the \( s' \) state as the pairing symmetry of the FeAs superconductors. We solve the Bogoliubov-de Gennes (BdG) equation self-consistently to calculate LDOS of the \( \pi \) state superconductor/normal metal (S/N) bilayers. It will be demonstrated that the observed zero bias conductance peaks which seemed difficult to understand with a fully gapped pairing state may be consistently understood within the \( s' \) pairing state.

**Model** – The FeAs superconductors have the disconnected electron and hole Fermi surfaces. A minimal model has to include two bands; a hole band around the \( \Gamma = (0, 0) \) point and an electron Fermi surface around the \( M = (\pi, \pi) \) point \[32\]. We write the BdG equation for S/N bilayers with two band superconductivity as

\[
H = H_S + H_N + H_{int},
\]

\[
H_S = \sum_{n,k,\sigma} \sum_{1 \leq y \leq y_S} \xi_{nk} c_{n\kappa \sigma}^\dagger(y) c_{n\kappa \sigma}(y) + \sum_{n,k,\sigma} \left[ \Delta_{nk}(y) c_{n\kappa \sigma}^\dagger(y) c_{n',-k \sigma}(y) + h.c. \right]
\]

\[
- t_0 \sum_{n,k,\sigma} \sum_{1 \leq y \leq y_S} \left[ a_{n\kappa \sigma}^\dagger(y) a_{n\kappa \sigma}(y) (y + 1) + h.c. \right] ,
\]

\[
H_N = \sum_{k,\sigma} \sum_{y_S + 1 \leq y \leq y_N} \xi_{kk} c_{k\kappa \sigma}^\dagger(y) a_{k\kappa \sigma}(y) + \sum_{k,\sigma} \left[ a_{k\kappa \sigma}^\dagger(y) a_{k\kappa \sigma}(y) (y + 1) + h.c. \right] ,
\]

\[
H_{int} = -t_1 \sum_{k,\sigma} \left[ c_{k\kappa \sigma}^\dagger(y_S) a_{k\kappa \sigma}(y_S + 1) + h.c. \right] + t_2 \sum_{k,\sigma} \left[ c_{k\kappa \sigma}^\dagger(y_S) a_{k\kappa \sigma}(y_S + 1) + h.c. \right] .
\]

Here, the subscript \( n = 1 \) and \( 2 \) refer to the hole and electron Fermi surfaces around the \( \Gamma \) and \( M \) points in the momentum space, respectively. \( k \) is the intra-layer crystal momentum in the \( z-x \) plane. \( y \) is perpendicular to the interface between S and N. \( y_S \) and \( y_N \) are thickness of S and N layers, respectively, in the unit of the distance between neighboring single layers, and \( y_t = y_S + y_N \). \( a \), \( c_1 \), and \( c_2 \) are the electron operators for the N, the hole band, and the electron band of S, respectively. The self-consistency relation for the gap function \( \Delta_{nk}(y) \) is given by

\[
\Delta_{nk}(y) = \sum_{n',k'} V(n,k;n',k') \langle c_{n',-k' \sigma}(y) c_{n'k' \sigma}^\dagger(y) \rangle ,
\]

where \( V(n,k;n',k') = V_{nn'} \) is the pairing interaction.

Let us first consider bulk s-wave two band BCS superconductivity. Putting \( V_{ij} N_j = \lambda_{ij} \), where \( N_1 \) and \( N_2 \) are the DOS per spin at the Fermi level for the band 1 and 2, respectively, Eqs. (2) and (3) are reduced to \[24,31\]

\[
\Delta_1 = \lambda_{11} F(\Delta_1) \Delta_1 + \lambda_{12} F(\Delta_2) \Delta_2 ,
\]

where \( F(\Delta) \) is given by

\[
F(\Delta) = \int_0^{2\pi} d\xi \frac{1}{E} \tanh \left( \frac{1}{2} E \right) , \quad E = \sqrt{\xi^2 + \Delta^2} \quad (7)
\]

At \( T = T_c \), \( F = \ln(1.14\omega_D/T_c) \). The \( T_c \) is the highest temperature where the larger eigenvalue of Eq. (6) becomes 1.

To see physics through more clearly, consider the simplest case of \( \lambda_{11} = \lambda_{22} = \lambda \) and \( \lambda_{12} = \lambda_{21} = \lambda' \). The single band BCS expression for the critical temperature \( T_c = 1.14\omega_D e^{-1/\lambda} \) is now replaced by one of the two expressions:

\[
T_c = 1.14\omega_D e^{-1/(\lambda+\lambda')}, \quad \lambda' < 0 \quad (8)
\]

\[
T_c = 1.14\omega_D e^{-1/(\lambda-\lambda')}, \quad \lambda' > 0 \quad (9)
\]

For \( \lambda' < 0 \), Eq. (9) is the appropriate expression, and the pairing order parameter \( \Delta_1 \) and \( \Delta_2 \) on the two bands acquire the \( \pi \) phase shift, which is the case considered here. The negative pairing interaction in one band BCS theory does not permit superconductivity. For the two band case, however, the negative interaction is turned to induce pairing by generating the sign reversal between \( \Delta_1 \) and \( \Delta_2 \) as can easily be seen from Eq. (6). The physical nature of the negative interaction parameterized in terms of \( \lambda' \) we do not specify here, although it is most likely due to the antiferromagnetic fluctuations with a peak around the momentum transfer \( Q = (\pi, \pi) \) \[17,24,33,36\].

The simple result of \( |\Delta_1| = |\Delta_2| \) is an accidental consequence of the simple parameterization of \( \lambda_{11} = \lambda_{22} \) and \( \lambda_{12} = \lambda_{21} \). For more realistic parameterizations of the pairing interaction, the magnitudes of the two gaps are different and additional peaks show up in LDOS as shown in Fig. 2 below. One of many interesting consequences of the \( s' \pi \) state is that the magnitude of one gap in general is larger than the BCS value while the other gap is smaller, that is, \( 2|\Delta_1|/T_c > 3.52 \) and \( 2|\Delta_2|/T_c < 3.52 \). Another, perhaps more interesting feature of the \( s' \) pairing state is the appearance of the zero bias peak which may be probed experimentally by the tunneling spectroscopy. Szabo et al. recently performed directional point contact Andreev reflection spectroscopy on \( (\text{BaO}_{0.55} \text{K}_{0.45})\text{Fe}_2 \text{As}_2 \) and found that some of the \( ab \) plane spectra reveal the zero-bias conductance peak consistent with the present work \[37\].

**LDOS of S/N bilayers** – Now, consider the S/N bilayers of the \( s' \pi \) pairing state described by Eq. (11) of the thickness \( y_t = y_S + y_N \). The Hamiltonian is written as an \( M \times M \) matrix, where \( M = 4y_S + 2y_N \), on the basis of \( \Psi \), which is taken as

\[
\Psi_k^\dagger = \left( c_{1k\uparrow}(1), c_{1,-k\downarrow}(1), c_{2k\uparrow}(1), c_{2,-k\downarrow}(1), c_{1k\downarrow}(2), c_{1,-k\uparrow}(2), \cdots, a_{k\uparrow}(y_t), a_{k\downarrow}(y_t) \right) .
\]
We first took the simple parameterization of \( \lambda = 0, \lambda' = -0.8, t_0 = t_1 = t_2 = 0.25 \) in the unit of the Fermi energy \( E_F \). With the parameterization, we diagonalized the \( M \times M \) matrix and calculated the gap function using Eq. \( (5) \). This procedure was repeated until the self-consistency was reached. In Fig. 1(a) we show the zero temperature 3 dimensional perspective plot of the LDOS of an S/N bilayer of 20 S layers and 20 N layers as a function of energy in the unit of the bulk pairing amplitude, \( V/\Delta_0 \). The ratio of the gap to the Fermi energy in bulk, \( \Delta_0/E_F \), is 0.053. The coherence length in the unit of inter-layer distance is then \( \xi_S \approx 3 - 4 \) and the thickness of S layer is large enough to monitor the evolution of the proximity effects as one moves away from the S/N interface. Notice the LDOS enhancement in the subgap energy region near the interface. The origin of this zero bias enhancement is the sign change of the order parameter. This point becomes clearer when we compare the present results with a two gap superconductor of the same sign.

\[
\begin{align*}
\lambda' = 0 \\
t_0 = t_1 = t_2 = 0.25 \\
\lambda = 0
\end{align*}
\]

FIG. 1: (a) A 3D plot of LDOS of an \( s\pi \) state S/N bilayer with \( \Delta_1 = -\Delta_2 \) as a function of \( V/\Delta_0 \) and the layer index. Notice the enhancement of the DOS in the subgap region near the interface due to the sign reversal of the order parameter. (b) The same as (a) but with \( \Delta_1 = \Delta_2 \). The LDOS behaves exactly as the well established conventional S/N bilayers.

For comparison we repeated the same calculations as (a) with all the parameters remain unchanged except that the interband pairing interaction is turned to a positive \( \lambda' = 0.8 \), corresponding to the case of Eq. \( (5) \). In this case, \( \Delta_1 = \Delta_2 \), and the LDOS should show the usual S/N behavior as shown in Fig. 1(b). The expected proximity effects are seen in the S and N regions. Compare this with the much short ranged proximity effects in the N layers of Fig. (a). The proximity effects of \( \Delta_1 \) and \( \Delta_2 \) for the \( s\pi \) pairing state cancel each other almost exactly other than the zero bias enhancement around the interface of S/N bilayers because they have the opposite sign and equal amplitude.

The subgap enhancement is a robust feature of an \( s\pi \) state. It is a manifestation of the phase shift of \( \pi \) between the two condensates which is insensitive to parameters. To demonstrate this we show in Fig. 2 the results of more realistic parameterization. We took \( \lambda_1 = 0.1, \lambda_2 = 0.2, \lambda_12 = -1.0, \lambda_21 = -0.5, t_0 = 0.25, \) and \( t_1 = t_2 = 0.2 \). As discussed above, other than another gap feature shows up inside the larger gap, the zero bias enhancement can clearly be seen. For the S/F \( \pi \) state, the subgap enhancement was observed for appropriate thickness of F where the order parameter changes its sign, referred to also as DOS reversal \[31\]. For the \( d \)-wave pairing case, the sign change of the order parameter occurs along the \((110)\) surface, and the zero bias conductance peak was also predicted and observed in the cuprate superconductors \[38, 39, 40\]. For \( s\pi \) state the peak appears unless one of \( t_1 \) and \( t_2 \) is negligible such that both condensates are probed.

**Summary and outlook** – We presented the local density of states of an S/N bilayer based on a generic two band superconductivity model with the internal \( \pi \) phase. The sign change of the pairing order parameter induced the LDOS enhancement in the subgap region near the interface as was observed by various tunneling spectroscopy on the FeAs superconductors. Some of the experiments, however, exhibit much sharper conductance peaks. This zero bias peak may be understood by more realistic extensions of the present work. Dictated by the Hamiltonian of Eq. \[11\], an electron of the intra-layer momentum \( k \) tunneled from the N side may encounter the hole and electron band pairing gaps with the amplitudes \( t_1 \) and \( t_2 \), respectively. More realistically, however, the specularly reflected electron and Andreev reflected hole may pick up the coherent phase difference of \( \pi \) if their intra-layer momenta fall on the electron and hole Fermi surfaces, respectively. This process, which has been included on an average manner in the present work, can produce a much sharper conductance peak as observed in the pnictides and along the \((110)\) surface of the cuprates.

Other realistic considerations will be to allow the hopping amplitudes of the electron and hole bands with the N layers, \( t_1 \) and \( t_2 \), to be different, or to consider more realistic pairing interactions. When these extensions are included, the LDOS will show more diverse and intriguing behavior. Also interesting will be the spectroscopy of
FIG. 2: The LDOS of an \( \pi \) state S/N bilayer with \(|\Delta_1| \neq |\Delta_2|\). The blue and red curves are LDOS in the S and N layers, respectively. Each curve represents the LDOS of each layer and is shifted upward for clarity. Notice the enhancement of the DOS in the subgap region near the interface due to the sign reversal of the order parameter.

other kinds of \( \pi \) state multilayers. For instance, the S/F bilayers with the \( s\pi \) state will exhibit intriguing interplay between the internal and external \( \pi \) phases. The works on these topics are in progress.

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[1] Y. Kamihara et al., J. Am. Chem. Soc. 128, 10012 (2006).
[2] Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono, J. Am. Chem. Soc. 130, 3296 (2008).
[3] Phys. Today 61, Issue 5, 11 (2008).
[4] G. F. Chen, Z. Li, D. Wu, G. Li, W. Z. Hu, J. Dong, P. Zheng, J. L. Luo, and N. L. Wang, Phys. Rev. Lett. 100, 247002 (2008).
[5] X. H. Chen, T. Wu, G. Wu, R. H. Liu, H. Chen, and D. F. Fang, Nature 453, 761 (2008).
[6] C. de la Cruz, Q. Huang, J. W. Lynn, J. Li, W. Ratcliff II, J. L. Zarestky, H. A. Mook, G. F. Chen, J. L. Luo, N. L. Wang, P. Dai, Nature 453, 899 (2008).
[7] M. Rotter, M. Tegel, and D. Johrendt, arXiv:0805.4630 (2008).
[8] H. Ding, P. Richard, K. Nakayama, T. Sugawara, T. Arakane, Y. Sekiba, A. Takayama, S. Souma, T. Sato, T. Takahashi, Z. Wang, X. Dai, Z. Fang, G. F. Chen, J. L. Luo, and N. L. Wang, Europhys. Lett. 83, 47001 (2008).
[9] L. Zhao et al., arXiv:0807.0398.
[10] T. Kondo, A. F. Santander-Syro, O. Copie, C. Liu, M. E. Tillman, E. D. Mun, J. Schmalian, S. L. Bud’ko, M. A. Tanatar, P. C. Canfield, and A. Kaminski, arXiv:0807.0815.
[11] C. Martin, R. T. Gordon, M. A. Tanatar, M. D. Vannette, M. E. Tillman, E. D. Mun, P. C. Canfield, V. G. Kogan, G. D. Samolyuk, J. Schmalian, and R. Prozorov, arXiv:0807.0876.
[12] G. Li, W. Z. Hu, J. Dong, Z. Li, P. Zheng, G. F. Chen, J. L. Luo, and N. L. Wang, arXiv:0807.1094.
[13] K. Matano, Z.-A. Ren, X. L. Dong, L. L. Sun, Z. X. Zhao, and G.-q. Zheng, arXiv:0806.0249.
[14] H.-J. Grafe, D. Paar, G. Lang, N. J. Curro, G. Behr, J. Werner, J. Hamann-Borrero, C. Hess, N. Leps, R. Klinger, and B. Buechner, arXiv:0805.2595.
[15] Y. Nakai, K. Ishida, Y. Kamihara, M. Hirano, and H. Hosono, arXiv:0804.4755.
[16] H. Mukuda, N. Terasaki, H. Kinouchi, M. Yashima, Y. Kitaoka, S. Suzuki, S. Miyassaka, S. Tajima, K. Miyazawa, P. M. Shirage, H. Kito, H. Eissaki, and A. Iyo, arXiv:0806.3238.
[17] A. D. Christianson, E. A. Goremychkin, R. Osborn, S. Rosenkranz, M. D. Lumsden, C. D. Malliakas, I. S. Todorov, H. Claus, D. Y. Chung, M. G. Kanatzidis, R. I. Bewley, and T. Guidi, arXiv:0807.3932.
[18] T. Y. Chen, Z. Tesanovic, R. H. Liu, X. H. Chen, and C. L. Chien, Nature 453, 1224 (2008).
[19] G. E. Blonder, M. Tinkham, and T. M. Klapwijk, Phys. Rev. B 25, 4515 (1982).
[20] L. Shan, Y. Wang, X. Zhu, G. Mu, L. Fang, and H.-H. Wen, arXiv:0803.2405.
[21] Y. Wang, L. Shan, L. Fang, P. Cheng, C. Ren, and H.-H. Wen, arXiv:0806.1986.
[22] O. Millo, I. Asulin, O. Yuli, I. Felner, Z.-A. Ren, X.-L. Shen, G.-C. Che, and Z.-X. Zhao, arXiv:0807.0350.
[23] P. Samuely, P. Szabo, Z. Pribulova, M. E. Tillman, S. Bud’ko, and P. C. Canfield, arXiv:0806.1672.
[24] I. I. Mazin, D. J. Singh, M. D. Johannes, and M. H. Du, Phys. Rev. Lett. 101, 057003 (2008).
[25] D. Parker, O. V. Dolgov, M. M. Korshunov, A. A. Golubov, and I. I. Mazin, arXiv:0807.3729.
[26] A. V. Chubukov, D. Efremov, and I. Eremin, arXiv:0807.3735.
[27] K. Kuroki, S. Onari, R. Arita, H. Usui, Y. Tanaka, H. Kontani, and H. Aoki, arXiv:0803.3325.
[28] A. G. Aronov and E. B. Sonin, Zh. Eksp. Teor. Fiz. 44, 1059 (1963) [Sov. Phys. JETP 36, 556 (1973)].
[29] M. J. Rice, H. Y. Choi, and Y. R. Wang, Phys. Rev. B 44, 10414 (1991).
[30] E. A. Demler, G. B. Arnold, and M. R. Beasley, Phys. Rev. B 55, 15174 (1997).
[31] T. Kontos, M. Aprili, J. Lesueur, and X. Grison, Phys. Rev. Lett. 86, 304 (2001).
[32] The zero bias peak due to the order parameter sign change has a deep root founded on the Atiyah-Singer index theorem.
[33] S. Raghu, X.-L. Qi, C.-X. Liu, D. Scalapino, and S.-C. Zhang, Phys. Rev. B 77, 220503(R) (2008).
[34] H. Suhl, B. T. Matthias, and L. R. Walker, Phys. Rev.
Lett. 3, 552 (1959).
[35] Y. Bang and H.-Y. Choi, arXiv:0807.3912.
[36] The sign reversal between the condensates means that the interband pairing must be repulsive, that is, \( \lambda_{12}, \lambda_{21} < 0 \). This observation eliminates the phonon and leaves the Coulomb repulsion of both charge and spin channels for the pairing interaction. Together with this, the observations that the two bands are separated by the \( \vec{Q} = (\pi, \pi) \) and the spin susceptibility has a peak also around \( \vec{Q} \) strongly hint that the antiferromagnetic fluctuations act as the pairing glue.
[37] P. Szabo, Z. Pribulova, G. Pristas, S. L. Budko, P. C. Canfield, and P. Samuely, arXiv:0809.1566.
[38] C. R. Hu, Phys. Rev. Lett. 72, 1526 (1994).
[39] J. Y. T. Wei, N.-C. Yeh, D. F. Garrigus, and M. Strasik, Phys. Rev. Lett. 81, 2542 (1998).
[40] H.-Y. Choi, Y. Bang, and D. K. Campbell, Phys. Rev. B 61, 9748 (2000).