Nodal gap structure of BaFe$_2$(As$_{1-x}$P$_x$)$_2$ from angle-resolved thermal conductivity in a magnetic field

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The fundamental mechanism that causes high-temperature superconductivity is a central issue in the physics of Fe-pnictides. Knowledge of the superconducting (SC) gap structure is a major step toward identifying the interactions that produce pairing. However, despite tremendous experimental and theoretical efforts, the SC gap structure remains one of the most controversial topics in these materials. The Fe-pnictides have several electron and hole bands and the interband interaction is very important for superconductivity. Nesting between electron and hole bands promotes antiferromagnetism and the $s_{\pm}$-wave gap symmetry with a sign change between nested bands. In contrast, orbital fluctuations promote an $s_{++}$ gap without a sign change.

Recent experiments revealed that several Fe-pnictide superconductors have line nodes in the SC gap. They include LaFePO ($T_c \approx 6$ K) and KFe$_2$As$_2$ ($T_c \approx 3$ K) and BaFe$_2$(As$_{1-x}$P$_x$)$_2$. The presence of line nodes in the latter material is especially intriguing because the transition temperature of this system in the optimally doped region, $T_c = 31$ K at $x = 0.33$, is comparable to the highest $T_c$ of hole-doped (Ba$_{1-x}$K$_x$)Fe$_2$As$_2$ ($T_c = 37$ K) whose Fermi surface (FS) is fully gapped in the SC state. In BaFe$_2$(As$_{1-x}$P$_x$)$_2$, substitution of isoelectronic P for As suppresses the magnetic order and induces superconductivity without charge doping. This system is very clean as demonstrated by the observed quantum oscillations and by the low critical current density in the vortex state. In addition, the $x$-dependence of several physical quantities is consistent with a quantum critical point near the boundary of magnetism and superconductivity. Therefore this system is suitable for studying the intrinsic nature of the high-$T_c$ superconductivity and for determining the detailed SC gap structure.

Here we report angle-resolved measurements of the thermal conductivity $\kappa$ in a rotated magnetic field $\mathbf{H}$, which is a bulk probe of the position of the gap nodes in unconventional superconductors. We observed distinct fourfold modulations under field rotation within the $ab$ plane. Combined with the results of the superfluid density $\rho_s$, a specific heat $C_p$, the band structure calculation and guided by comparison with the theoretical predictions for angular variations of $\kappa$ for different FS shapes and nodal structures, we conclude that the nodal lines form closed loops at the flatter part of the electron Fermi surface with high Fermi velocity.
field. Previous $\kappa/T$($T$, $H$) and $\rho_s(T)$ measurements already indicate the presence of nodes rather than the gap minima, so we focus solely on the location of the nodes. The strength of the pair breaking in a given near-nodal region vanishes if we focus solely on the location of the nodes. The strength of the pair breaking in a given near-nodal region vanishes if we focus solely on the location of the nodes.

The above analysis also suggests that the nodes may be located in the flat parts in the outer electron sheets, where the Fermi velocity is highest. Indeed, Figs. 2(b), and 2(c) depict $\kappa/T$($H$) also have a higher Doppler shift implying little change in $v_F$ at the near-nodal regions. Finally, in an applied field the residual $\kappa/T$ exhibits a clear $\sqrt{H}$ dependence over a much wider range than the residual specific heat $C/T$, which looks nearly linear above $5T$. This suggests that the nodes are located in regions with higher in-plane Fermi velocity $v_F^{ab}$, as those give a lower relative contribution to $C/T$ [proportional to the density of states, DOS, $N(\varepsilon_F, H)$] than to transport [proportional to $N(\varepsilon_F)(v_F^{ab})^2$. The shading of Fig. 2(a) represents the magnitude of $v_F^{ab}$ with the red (blue) area denoting regions with high (low) Fermi velocity. It is clear that the hole pockets have low velocity and heavy mass quasiparticles, while the electron FS sheets have high velocity and light mass. Considering that the electron pockets have a lower scattering rate than the hole pockets, their contribution to the total thermal conductivity is even more pronounced. Note that these regions with high $v_F^{ab}$ also have a higher Doppler shift $\Delta \varepsilon$ for $H \perp ab$. Together, these observations strongly support the scenario with the nodes on the electron sheet.

The first question is at which FS(s) are the nodes located. We believe that the nodes are on the electron sheets. First, recent bulk-sensitive laser angle-resolved photoemission spectroscopy (ARPES) experiments report isotropic gaps in all three hole pockets around Z point. This by itself excludes the $d$-wave gap symmetry and we focus on the $A_{1g}$ representation. Second, there are significant changes in the shape of the hole FSs with $x$ in BaFe$_2$(As$_{1-x}$P$_x$)$_2$, while the shape of the electron surfaces remains nearly the same. The slope of the $T$-linear penetration depth, indicative of robust line nodes, simply scales with $T_c$ in a wide range of $x$ implying little change in $v_F$ at the near-nodal regions.
ther explore the nodal locations. The fourfold oscillations of κ(φ) of similar amplitude to that in materials with vertical line nodes argue against nearly horizontal line nodes suggested by several theories.\(^{26,27}\) Depending on the temperature and field range either minima or maxima of κ_{\parallel,\phi} can indicate nodal directions.\(^{18}\) The inversion of the oscillations reported in Fe(Se,Te) with a similar FS structure\(^{24}\) occurs at a much higher temperature and field than our range (0.03 ≤ T/T_c ≤ 0.13 and 0.007 ≲ H/H_{c2} ≲ 0.06). Therefore the minima at φ = ±45° observed in our low-T and low-H range indicate that the nodes are located at the position of the FS where v_F is nearly parallel to [±1, ±1, 0] directions.

In the A_{1g} symmetry we consider three possible nodal structures shown in Figs. 3(a)–3(c): (a) eight vertical line nodes, (b) closed loop line nodes in the flat part\(^{20}\) and (c) nodal loops in the high curvature part. To distinguish between those possibilities we compute the profile of the thermal conductivity as a function of the field angle using the microscopic approach of Ref.\(^{18}\) generalized to the multiband system in Ref.\(^{22}\), which has been successful in describing C/T and κ/T oscillations on equal footing. We take one electron and one hole FS, assume the hole FS to be fully gapped, and consider a nodal order parameter on the electron sheet.

An intuitive physical analysis connects the smallness of the twofold term with the nodes in the flat part of the ellipse—see Figs. 3(d)–3(g). The two ellipsoids represent the electron sheets at (π, π) and (π, π) points respectively. Recall that quasiparticles are predominantly generated at locations where v_F \perp H (filled red circles), and quasiparticles with v_F \parallel q contribute more to the heat transport. If the nodes are in the high curvature region (in the case of Fig. 3(c)), the Fermi velocities at the nodes are not parallel. For the field parallel (normal) to the heat current, the majority of unpaired states have v_F nearly normal (parallel) to the heat current [Figs. 3(f), (g)] yielding a dominant twofold component [see the red curve in Fig. 3(h)]. In contrast, the nodes on the flat part of the ellipse [in the case of Fig. 3(b)] have a nearly identical direction of the Fermi velocity [Figs. 3(d), and 3(e)], and contribute equally to the q for both H∥q and H \perp q [see the black curve in Fig. 3(h)]. Thus our observation that a large fourfold component dominates over the twofold one showing clear minima near ±45° eliminates the possibility of the nodal loops at the sharp edges of the FS (Fig. 3(c)). It also argues against vertical line nodes [Fig. 3(a)] as this order parameter structure would essentially average the two curves in Fig. 3(h), leaving a large twofold anisotropy\(^{18}\) not seen in our experiment.

To confirm that the nodal loops as sketched in Fig. 3(b) consistently describe the bulk of the experimental measurements, we performed calculations for a three-dimensional (3D) FS given by 2mE_f \propto (k_z a)^2/(1 - \mu \cos k_x a) + (k_y a)^2/(1 + \mu \cos k_y a). For \mu = 0.5 the FS closely mimics what obtained in the band structure calculations. We took the order parameter in the form \Delta = \Delta_x Y(\phi, k_z), where Y(\phi, k_z) = 1 - |r\!(k_z)| + r\!(k_z) \cos 2\phi, and r\!(k_z) = -0.6 \cos k_z/2. We
also took the hole FS to be cylindrical with an isotropic gap $\Delta_h$, and self-consistently determined both $\Delta_o(T, H)$ and $\Delta_h(T, H)$ assuming a dominant interband pairing interaction. Figure 4 shows that within this framework we can explain all the salient experimental features: linear-in-$T$ penetration depth, a large residual term in the thermal conductivity, and the dominant fourfold profile of $\kappa(\phi)$ under rotated field with a minimum along the 45° direction. We therefore believe that this is the most likely location of the gap nodes in BaFe$_2$(As$_{0.67}$P$_{0.33}$)$_2$.

Finally we discuss why such a nodal loop structure is realized. Experimentally, recent neutron scattering measurements suggest that the line nodes should create only a limited area of sign-reversal on a single FS, which is consistent with the present nodal loop structure. The Raman scattering in Ba(Fe,Co)$_2$As$_2$ suggested a similar loop structure of gap minima. A number of model calculations predict that the superconducting gap in the electron FSs can be more anisotropic than that in hole bands, and that nodes can appear in some part of the electron FS regions with low DOS does not significantly reduce the SC condensation energy. In addition, it has been suggested that the nesting between the FS regions with the same orbital character is important for the pairing interaction. We note that the change of the orbital character from $xy$ to $xz+yz$ occurs near the rim of the flat part of the electron pocket, implying that the orbital character may favor the closed-loop nodes. Thus the pairing interaction and low DOS stabilize the nodal loop structure with no serious reduction of $T_c$. A more detailed fully microscopic calculation is required to clarify the origin of the closed nodal loop structure, which is unique among unconventional superconductors.

In summary, we determined the nodal gap structure of BaFe$_2$(As$_{0.67}$P$_{0.33}$)$_2$ by angle-resolved thermal conductivity measurements. We found distinct fourfold oscillation in $\kappa(\phi)$ with minima at $[\pm 1, \pm 1, 0]$ directions. The observed results are most consistent with the closed nodal loops at the flat part of the electron FS.

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1. J. Paglione and R. L. Greene, Nat. Phys. 6, 645 (2010).
2. I. I. Mazin, D. J. Singh, M. D. Johannes, and M. H. Du, Phys. Rev. Lett. 101, 057003 (2008).
3. K. Kuroki, H. Usui, S. Onari, R. Arita, and H. Aoki, Phys. Rev. B 79, 224511 (2009).
4. H. Kontani and S. Onari, Phys. Rev. Lett. 104, 157001 (2010).
5. J. Fletcher et al., Phys. Rev. Lett. 102, 147001 (2009).
6. M. Yamashita et al., Phys. Rev. B 80, 220509(R) (2009).
7. K. Hashimoto et al., Phys. Rev. B 82, 014526 (2010).
8. K. Hashimoto et al., Phys. Rev. B 81, 220501(R) (2010).
9. Y. Nakai et al., Phys. Rev. B 81, 020503(R) (2010).
10. S. Kasahara et al., Phys. Rev. B 81, 184519 (2010).
11. K. Hashimoto et al., Phys. Rev. Lett. 102, 207001 (2009).
12. H. Ding et al., EPL 83, 47001 (2008).
13. H. Shishido et al., Phys. Rev. Lett. 104, 057008 (2010).
14. C. J. van der Beek et al., Phys. Rev. Lett. 105, 267002 (2010).
15. Y. Nakai et al., Phys. Rev. Lett. 105, 107003 (2010).
16. I. Vekhter, P. J. Hirschfeld, J. P. Carbotte, and E. J. Nicol, Phys. Rev. B 59, R9023 (1999); C. Kübert and P. J. Hirschfeld, Phys. Rev. Lett. 80, 4963 (1998).
17. Y. Matsuda, K. Izawa, and I. Vekhter, J. Phys.: Condens. Matter 18, R705 (2006).
18. A. Vorontsov and I. Vekhter, Phys. Rev. Lett. 96, 237001 (2006); Phys. Rev. B 75, 224502 (2007).
19. S. Graser et al., Phys. Rev. B 77, 180514(R) (2008).
20. A. V. Chubukov and I. Eremin, Phys. Rev. B 82, 060504(R) (2010).
21. B. Zeng et al., Nat. Commun. 1, 112 (2010).
22. A. B. Vorontsov and I. Vekhter, Phys. Rev. Lett. 105, 187004 (2010).
23. J. S. Kim et al., Phys. Rev. B 81, 214507 (2010).
24. T. Shimojima et al., Science 332, 564 (2011).
25. K. Hashimoto et al. (unpublished).
26. S. Graser et al., Phys. Rev. B 81, 214503 (2010).
27. K. Suzuki, H. Usui, and K. Kuroki, J. Phys. Soc. Jpn. 80, (2011).
28. R. Thomale, C. Platt, W. Hanke, and B. A. Bernevig, Phys. Rev. Lett. 106, 187003 (2011).
29. A. V. Chubukov, M. G. Vavilov, and A. B. Vorontsov, Phys. Rev. B 80, 140515 (2009).
30. A. Y. Ferreira et al., Phys. Rev. B 82, 180502(R) (2010).
31. V. Mishra, A. Vorontsov, P. J. Hirschfeld, and I. Vekhter, Phys. Rev. B 80, 224525 (2009).
32. M. Ishikado et al., arXiv:1011.3191.