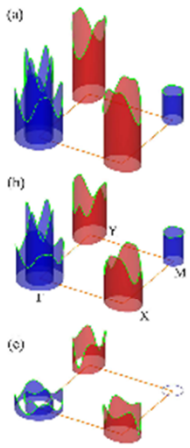
Calculations Reveal the Nature of Exotic Electron Pairing States in an Iron-based Superconductor



The superconducting band gap (red = positive, blue = negative) calculated in a microscopic spin-fluctuation model for the iron-based superconductors (a). Both normal pairing (b) and eta-pairing (c) contributions have even parity.

Work was performed at the Center for Nanophase Materials Sciences, ORNL

Scientific Achievement

Microscopic calculations of an iron-based superconductor demonstrate that exotic eta-pairs with finite center of mass momentum contribute to the superconducting condensate with even parity and time reversal symmetry.

Significance and Impact

This establishes the conventional even parity and time-reversal symmetric nature of singlet pairs in iron-based superconductors.

Research Details

- Studied the effects of the glide-plane symmetry of the Fe-pnictogen/chalcogen layer in Fe-based superconductors.
- Showed that eta-pairing with nonzero total momentum occurs naturally in these systems but contributes with the usual even parity and time reversal symmetry.
- Concluded that 1 Fe unit cell calculations can correctly predict the gap function that appears in physical observables.

Y. Wang, et al. *Physical Review Letters* 114, *107002* (2015), DOI: 10.1103/PhysRevLett.114.107002

U.S. DEPARTMENT OF ENERGY | Office of Science

UF UNIVERSITY of FLORIDA · THE UNIVERSITY of TENNESSEE KNOXVILLE · OAK RIDGE National Laboratory

Narrative Highlight Text:
This work uses concrete and realistic microscopic calculations for 2-Fe and 1-Fe models of iron-based superconductors to demonstrate that earlier 1-Fe calculations correctly accounted for this glide-plane symmetry and correctly predicted its implications on the observable superconducting gap. It furthermore shows that eta-pairing naturally arises in systems where both orbitals with even and orbitals with odd mirror reflection symmetry in z contribute to the Fermi surface states. In contrast to the recent proposals, however, this study finds that eta-pairing contributes with the usual even parity symmetry and that time reversal symmetry is not broken. This work establishes a clear framework for the study of such questions in other unconventional superconductors.

Reference

"Glide-Plane Symmetry and Superconducting Gap Structure of Iron-Based Superconductors"
Y. Wang,[1,2,3] T. Berlijn,[1,4] P.J. Hirschfeld,[3] D.J. Scalapino,[5] T.A. Maier[1,4]
[1]Center for Nanophase Materials Sciences, ORNL, [2]Department of Physics and Astronomy, University of Tennessee, Knoxville [3]Department of Physics, University of Florida, Gainesville, [4]Computer Science and Mathematics Division, ORNL, [5]Department of Physics, University of California, Santa Barbara
Physical Review Letters 114, *107002* (2015).

Acknowledgment of Support

P. J. H. and Y.W. were supported by Grant No. DOE DE-FG02-05ER46236, and T. B. was supported as a Wigner Fellow at the Oak Ridge National Laboratory. A portion of this research wasconducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy. This research was supported in part

by Kavli Institute for Theoretical Physics under National Science Foundation Grant No. PHY11-25915.