Theoretical/Computational Studies of High-Temperature Superconductivity from Quantum Magnetism

Jose Rodriguez
CALIFORNIA STATE UNIVERSITY AUXILIARY SERVICES INC

06/09/2016
Final Report

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**4. TITLE AND SUBTITLE**
Theoretical/Computational Studies of High-Temperature Superconductivity from Quantum Magnetism

**14. ABSTRACT**
The symmetry of a single Cooper pair in a monolayer of hole-doped or electron-doped iron superconductor was determined at the limit of strong on-site Coulomb repulsion, with only the 3d xz and the 3d yz iron orbitals included. Exact numerical diagonalization that exploited AFRL supercomputers, in addition to meanfield theory, find isotropic pairing on the electron Fermi surface pockets plus isotropic pairing of opposite sign on hole bands buried below the Fermi level. These results potentially account for the high-temperature superconductivity displayed recently by surface layers of iron selenide.

**15. SUBJECT TERMS**
quantum magnetism, HTS, superconductivity
Final Report: Theoretical/Computational Studies of High-Temperature Superconductivity from Quantum Magnetism

Jose P. Rodriguez

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Abstract

The symmetry of a single Cooper pair in a monolayer of hole-doped or electron-doped iron superconductor was determine at the limit of strong on-site Coulomb repulsion, with only the 3d_{xz} and the 3d_{yz} iron orbitals included. Exact numerical diagonalization that exploited AFRL supercomputers, in addition to meanfield theory, find isotropic pairing on the electron Fermi surface pockets plus isotropic pairing of opposite sign on hole bands buried below the Fermi level. These results potentially account for the high-temperature superconductivity displayed recently by surface layers of iron selenide.

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I. INTRODUCTION

Below, we describe the PI’s scientific activity funded by AFSOR grant no. FA9550-13-1-0118. The funding period began March 1, 2013, and it ended February 29, 2016. The PI devoted this funding cycle to uncovering the symmetry of Cooper pairs in a single layer of iron-pnictide/selenide superconductor at the limit of strong on-site Coulomb repulsion. Exact diagonalization techniques that exploited DoD supercomputers at the AFRL were brought to bear on the difficult many-electron problem that the PI was faced with. This, in conjunction with a meanfield analysis, revealed a new groundstate for surface-layers FeSe that potentially accounts for the high-temperature superconductivity that these systems show.

II. PUBLICATIONS AND PRESENTATIONS

A. Publications


B. Manuscripts in Preparation


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C. Presentations


2. J.P. Rodriguez, “Iron-pnictide High-Tc Superconductivity from the limit of Local Magnetic Moments” (invited talk), Southern California Condensed Matter Theory Meeting held at California State University Long Beach, April 12, 2013.


6. J.P. Rodriguez, “Collective Modes in Iron Superconductors from the Local Moment Limit” (contributed talk), KITP Program on Magnetism, Bad Metals and Superconductivity: Iron Pnictides and Beyond, held at KITP, University of California Santa Barbara, September 2 - November 21, 2014.

7. J.P. Rodriguez, “Collective Modes in Iron Superconductors from the Local Moment Limit” (invited talk), Department of Physics and Astronomy, University of Southern California, February 27, 2015.


9. J.P. Rodriguez, “Are the New Class of Iron-Pnictide Superconductors Doped Mott Insulators?” (invited talk), Department of Physics and Astronomy, California State
III. SCIENTIFIC VISITS

1. Invited to participate in the KITP Program on Magnetism, Bad Metals and Superconductivity: Iron Pnictides and Beyond, held at KITP, University of California Santa Barbara, September 2 - November 21, 2014.

2. Invited by Professor Stephan Haas for sabbatical visit at the Department of Physics and Astronomy, University of Southern California, April 1 - June 30, 2015.

IV. PRINCIPAL RESULT OF FUNDED RESEARCH

Recent experimental studies reveal high-temperature superconductivity in surface layers of iron selenide\(^1,2\). These include an FeSe mono-layer over various substrates\(^3-5\), intercalated FeSe\(^6,7\), and bulk FeSe dosed with alkali metals over the surface\(^8,9\). All of these systems share a common electronic structure: 2D electron Fermi surface pockets at the corners of the Brillouin zone. Unlike iron-pnictide superconductors, the 2D hole bands at the Brillouin zone center are buried entirely below the Fermi level. Furthermore, the critical temperatures in surface-layer FeSe superconductors lie inside the range 40 – 110 K, which is substantially higher than the range of critical temperatures in iron-pnictide superconductors. All surface-layer FeSe superconductors also show an isotropic gap on the electron Fermi surface pockets\(^10\). The experimental findings listed above strongly suggest that the high-temperature superconductivity shown by surface-layer FeSe is due to a new underlying groundstate.

Calculations based on density-functional theory (DFT) typically predict hole Fermi surface pockets at the Brillouin zone center\(^11\), which is counter to what is observed by angle-resolved photoemission (ARPES)\(^2,6,7,9,10\). The PI has recently shown that the buried hole bands shown at surface layers of FeSe can be understood instead as emergent phenomena. He includes only the \(3d_{xz}\) and \(3d_{yz}\) orbitals, along with strong on-site Coulomb repulsion. Proximity to hidden magnetic order yields electron Fermi surface pockets at the corners of the Brillouin zone and hole bands at the Brillouin zone center that lie entirely below the Fermi level\(^12\).

The PI’s theory also predicts isotropic Cooper-pair symmetry on the electron Fermi
surface pockets, in addition to remnant isotropic Cooper pairing of opposite sign on the buried hole bands. This state of affairs occurs at a quantum-critical point tuned by Hund coupling, at which $s$-wave and $d$-wave Cooper pairs become degenerate in energy. Given the failure of DFT to describe electronic structure in surface layers of FeSe, the PI's approach based on emergent hole bands is possibly the only viable theory at the moment that describes the high-temperature superconductivity displayed by these new systems.


7. X.H. Niu, R. Peng, H.C. Xu, Y.J. Yan, J. Jiang, D.F. Xu, T.L. Yu, Q. Song, Z.C. Huang,


1. Report Type
Final Report

Primary Contact E-mail
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Primary Contact Phone Number
Contact phone number if there is a problem with the report
323-343-2133

Organization / Institution name
California State University at Los Angeles

Grant/Contract Title
The full title of the funded effort.
Theoretical/Computational Studies of High-Temperature Superconductivity from Quantum Magnetism

Grant/Contract Number
AFOSR assigned control number. It must begin with "FA9550" or "F49620" or "FA2386".
FA9550-13-1-0118

Principal Investigator Name
The full name of the principal investigator on the grant or contract.
Jose P. Rodriguez

Program Manager
The AFOSR Program Manager currently assigned to the award
Dr. Harold Weinstock

Reporting Period Start Date
03/01/2013

Reporting Period End Date
02/29/2016

Abstract
The symmetry of a single Cooper pair in a monolayer of hole-doped or electron-doped iron superconductor was determined at the limit of strong on-site Coulomb repulsion, with only the 3d \( xz \) and the 3d \( yz \) iron orbitals included. Exact numerical diagonalization that exploited AFRL supercomputers, in addition to meanfield theory, find isotropic pairing on the electron Fermi surface pockets plus isotropic pairing of opposite sign on hole bands buried below the Fermi level. These results potentially account for the high-temperature superconductivity displayed recently by surface layers of iron selenide.

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Changes in research objectives (if any):

Change in AFOSR Program Manager, if any:

Extensions granted or milestones slipped, if any:

AFOSR LRIR Number

LRIR Title

Reporting Period

Laboratory Task Manager

Program Officer

Research Objectives

Technical Summary

Funding Summary by Cost Category (by FY, $K)

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Report Document

Report Document - Text Analysis

Appendix Documents

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