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John S. Van Dyke

Electronic and Magnetic Excitations in Correlated and Topological Materials

Doctoral Thesis accepted by University of Illinois at Chicago, Chicago, Illinois, USA

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For my wife, Esther

Supervisor's Foreword

Understanding the complex properties of strongly correlated electron materials has been an outstanding problem at the forefront of research in condensed matter physics for nearly 40 years. It was stimulated by the discovery of the heavy fermion superconductors and the quest for identifying the microscopic mechanism responsible for the emergence of their unconventional superconducting phase. The similarity of the heavy fermion's phase diagram with that of subsequently discovered unconventional superconductors, such as the cuprate (high-temperature) or iron-based superconductors, has raised the question of a common, universal pairing mechanism. In particular, the proximity of the unconventional superconducting phase to antiferromagnetism in the phase diagram of all of these materials has given rise to the hypothesis of a pairing mechanism mediated by the exchange of antiferromagnetic fluctuations. For the heavy fermion materials, whose salient feature is a lattice of magnetic moments that are either Kondo screened by conduction electrons or ordered antiferromagnetically, this hypothesis has remained unproven despite an impressive body of theoretical and experimental studies. A major obstacle in verifying the hypothesis has been a lack of insight into the complex electronic and magnetic structure of these materials.

The work by Dr. John Van Dyke described in this book represents a major breakthrough in exploring and confirming this 30-year-old hypothesis for the heavy fermion material $CeCoIn_5$, considered to be a prototype material for the entire class of heavy fermion compounds. Dr. Van Dyke demonstrated—making use of recent groundbreaking quasiparticle interference (QPI) experiments by the group of Prof. J.C. Seamus Davis (Cornell University)—that characteristic signatures in the QPI spectrum of $CeCoIn_5$ can be employed to extract not only the momentum form of its superconducting order parameter—exposing its unconventional $d_{x2\text{-}y2}$-symmetry—but also the multi-band electronic structure crucial for the emergence of superconductivity. However, to quantitatively identify the microscopic pairing mechanism, a second crucial, and so far missing, element was necessary—the form of the superconducting pairing interaction that was proposed to arise from the antiferromagnetic coupling between the localized moments. Dr. Van Dyke showed that the momentum structure of this interaction can be extracted from the experimental QPI data, allowing him to develop a quantitative microscopic theory for the unconventional superconducting state in $CeCoIn_5$. This work resulted in seven predictions for this material's striking physical properties: the symmetry and momentum structure of the multi-band superconducting order parameter, the critical temperature, the momentum and energy dependence of the QPI as well as the phase-sensitive QPI spectrum, the temperature dependence of the spin-lattice relaxation rate, the energy position of the magnetic resonance peak, as well as the spatial form of the differential conductance around defects. The good quantitative agreement of these theoretical results with experimental measurements provided strong and direct evidence for the proposed mechanism underlying the unconventional superconducting state in heavy fermion materials.

Extending his work to investigate the nonequilibrium properties of heavy fermion materials, Dr. Van Dyke showed that the onset of Kondo screening and the ensuing changes in the electronic structure of the material significantly alter the spatial paths of currents flowing through heavy fermion systems. The considerable experimental advances in imaging the spatial flow of currents over the last few years have therefore opened a new venue for exploring the out-of-equilibrium signatures of strong correlation effects.

In the last part of his thesis, Dr. Van Dyke investigated the nonequilibrium charge transport in a new topological state of matter, the topological insulators (TIs), which are characterized by an insulating bulk, and gapless edge or surface modes. The topological nature of these materials renders their properties robust against many forms of disorder, making them of great interest for a whole range of technological applications in quantum computation and spin-based electronics. A major hurdle in the realization of these applications has been the lack of ability to independently create and control spin and charge currents at the nanoscale. Dr. Van Dyke showed that this obstacle can be overcome and that such control can be established by breaking the time-reversal symmetry of nanoscopic TIs via magnetic defects. This symmetry breaking does not only enable one to create nearly 100% spin-polarized charge currents, but it also allows for the design of novel spin diodes. The flow of spin and charge in these diodes can be controlled at the nanoscale by changing the gate and bias voltages, which provides the missing link in the use of TIs for technological applications. These results open unprecedented opportunities to employ nanoscale TIs for applications in spintronics and quantum information.

The study of topological and strongly correlated materials will continue to fascinate physicists for years to come, and Dr. Van Dyke's thesis provides a nice introduction into these exciting fields of research.

Chicago, IL, USA
October 2017

Dirk Morr

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Published Results and Contribution of Authors

Parts of this thesis have been published in the following journal articles:

[1]. M.P. Allan, F. Massee, D.K. Morr, J. Van Dyke, A.W. Rost, A.P. Mackenzie, C. Petrovic, J.C. Davis, Imaging Cooper pairing of heavy fermions in $CeCoIn_5$. Nat. Phys. **9**(8), 468–473 (2013)
[2]. J.S. Van Dyke, F. Massee, M.P. Allan, J.C.S. Davis, C. Petrovic, D.K. Morr, Direct evidence for a magnetic f-electron-mediated pairing mechanism of heavy-fermion superconductivity in $CeCoIn_5$. Proc. Natl. Acad. Sci. **111**(32), 11663–11667 (2014)
[3]. J.S. Van Dyke, J.C.S. Davis, D.K. Morr, Differential conductance and defect states in the heavy-fermion superconductor $CeCoIn_5$. Phys. Rev. B **93**(4), 041107 (2016)
[4]. Y. Song, J.V. Dyke, I.K. Lum, B.D. White, S. Jang, D. Yazici, L. Shu, A. Schneidewind, P. Čermák, Y. Qiu, M.B. Maple, D.K. Morr, P. Dai, Robust upward dispersion of the neutron spin resonance in the heavy fermion superconductor $Ce_{1-x}Yb_xCoIn_5$. Nat. Commun. **7**, 12774 (2016)
[5]. J.S. Van Dyke, D.K. Morr, Controlling the flow of spin and charge in nanoscopic topological insulators. Phys. Rev. B **93**(8), 081401 (2016)
[6]. J.S. Van Dyke, D.K. Morr, Effects of defects and dephasing on charge and spin currents in two-dimensional topological insulators. Phys. Rev. B **95**(4), 045151 (2017)

Chapter 1 is a brief introduction to the research areas considered in the thesis. Chapters 2 and 3 are based on [1] and [2]. C.P. synthesized and characterized the samples. M.P.A. and F.M. performed the STM experiments, prepared the data, and produced the published versions of the figures. J.V. and D.K.M. developed the band structure and superconducting gap models. J.V. performed the theoretical calculations discussed in the text. J.C.D. and D.K.M. supervised the projects. The manuscripts reflect the important contributions of all the authors. Chapter 4 is based on the manuscripts [3] and [4]. For [3], J.V. performed the calculations, D.K.M. supervised the project, and all the authors contributed to the writing of the manuscript. For [4], I.K.L., B.D.W., S.J., D.Y., L. Shu, and M.B.M. synthesized and characterized the samples. Y.S. performed the experiments with the assistance of A.S., P.C., and Y.Q., J.V. and D.K.M. developed the theoretical models; and J.V. performed the calculations. Y.S. prepared the data, and Y.S., J.V., and D.K.M.

produced figures. P.D. directed the project. Chapter 5 is based on unpublished work by J.V. and D.K.M., in which D.K.M. supervised the project and J.V. performed the calculations and produced the figures. Chapter 6 is based on the manuscripts [5] and [6]. J.V. and D.K.M. performed the calculations, and D.K.M. supervised the project and produced the published versions of the figures.