

北京大学量子材料科学中心

International Center for Quantum Materials, PKU

Weekly Seminar

How to predict the critical temperature of superconductors?



Eberhard K. U. Gross Max-Planck Institute of Microstructure Physics Halle (Saale), Germany

Time: 4:00 pm, Oct.30, 2013 (Wednesday)
时间: 2013年10月30日(周三)下午4:00
Venue: Conference Room A (607), No. 5 Science Building
地点: 理科五号楼607会议室

Abstract

A prominent challenge of modern condensed-matter theory is to predict reliably material-specific properties of superconductors, such as the critical temperature. The traditional model of Bardeen, Cooper and Schrieffer (BCS) properly describes the universal features that all conventional superconductors have in common, but it is not able to make accurate predictions of materialspecific properties. A novel density-functional-type approach to the description of phononmediated superconductivity is presented. The goal of this approach is to provide a theory with predictive power, allowing the calculation of material-specific properties such as the critical temperature. To this end, the electron-phonon interaction and the electron-electron repulsion are treated on the same footing. There are no adjustable parameters such as the μ^* of Eliashberg theory. Approximations of the universal xc functionals are derived on the basis of many-body perturbation theory. Numerical results for the critical temperature and the gap will be presented for simple metals, MgB₂, calcium intercalated graphite CaC₆, and for Li, Al and K under pressure. In particular, for MgB₂, the two gaps and the specific heat as function of temperature are in good agreement with experimental data. For Li and Al under pressure, the calculations explain why these two metals behave very differently, leading to a strong enhancement of superconductivity for Li and to a clear suppression for Al with increasing pressure. For fcc K we predict a behavior similar to Li, i.e. a strong increase of T_c with increasing pressure. Finally, results for hydrogen under extreme pressure will be presented. It turns out that hydrogen is a three-gap superconductor with a critical temperature of 242K at 450 Gpa.

About the Speaker

Prof. Eberhard K. U. Gross obtained his Ph.D. on Physics in 1980 from J.W.Goethe University. He was a Fiebiger Professor at University of Würzburg from 1990 to 2001, and a full professor of Theoretical Physics at the Free Universität Berlin from 2001 to 2009. Since then, he has been the director at the Max Planck Institute of Microstructure Physics, Halle(Saale). He has held many leading positions, such as President and German representative in the Council of Centre Eurepéen du Calcul Atomique et Moléculaire. Professor Gross received many honors and awards, including the Heisenberg Fellowship, Schlumberger Award, and elected Max Planck Fellow at the Fritz-Haber-Institut Berlin in 2005-2009.

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Host: 牛谦(niu@physics.utexas.edu)