MAR05-2004-006556

Abstract for an Invited Paper
for the MAR05 Meeting of
the American Physical Society

Denstity Functional Theory of Superconductivity[1]

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A novel density-functional approach to the description of phonon-mediated superconductivity is presented. The theory is formulated in terms of three quantities: the ordinary electron density, the superconducting order parameter, and the nuclear N-body density. These three "densities" are determined by a set of Bogoliubov-type Kohn-Sham equations representing the electronic degrees of freedom, and a Schrödinger equation with an N-body interaction describing the nuclear motion. These equations are coupled to each other via exchange-correlation (xc) potentials which are universal functionals of the three densities. The formalism can be viewed either as a strong-coupling generalization of the weak-coupling DFT for superconductors [1] or as a superconducting generalization of the multi-component DFT [2] for electrons and nuclei. Approximations of the universal xc functionals will be derived on the basis of many-body perturbation theory [3,4]. In this way, a true ab-initio description is achieved which does not contain any empirical parameters. Numerical results for the critical temperature and the gap will be presented for simple metals [5], for MgB_2 [6], and for Li and Al under pressure. In particular, for MgB_2, the two gaps and the specific heat as function of temperature are in very good agreement with experimental data. Moreover, our calculations show clearly, how the Coulomb interaction acts differently on σ and π states, thereby stabilizing the observed superconducting phase. 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.

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[1]work done in cooperation with the groups of S. Massidda, Cagliari, and A. Continenza, L'Aquila