Ab-initio theory of superconductivity: Density functional formalism, approximate functionals and first applications

M. Lüders[1,2], M. A. L. Marques[3,2], N. N. Lathiotakis[3,2], A. Floris[3,4], G. Profeta[5], L. Fast[6,2], A. Continenza[5], S. Massidda[4], E. K. U. Gross[3,2]

[1]*Daresbury Laboratory, Warrington WA4 4AD, United Kingdom*
[2]*Institut für Theoretische Physik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany*
[3]*Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany*
[4]*INFM SLACS, Sardinian Laboratory for Computational Materials Science and Dipartimento di Scienze Fisiche, Università degli Studi di Cagliari, S.P. Monserrato-Sestu km 0.700, I–09124 Monserrato (Cagliari), Italy*
[5]*C.A.S.T.I. - Istituto Nazionale Fisica della Materia (INFM) and Dipartimento di Fisica, Università degli studi dell'Aquila, I-67010 Coppito (L'Aquila) Italy*
[6]*SP Swedish National Testing and Research Institute, P.O.B. 857, S-501 15 Borås, Sweden*

Abstract

A novel approach to the description of superconductors in thermal equilibrium is developed within a formally exact density-functional framework. The theory is formulated in terms of three "densities": the ordinary electron density, the superconducting order parameter, and the diagonal of the nuclear N-body density matrix. The electron density and the order parameter are determined by Kohn-Sham equations that resemble the Bogoliubov-de Gennes equations. The nuclear density matrix follows from a Schrödinger equation with an effective N-body interaction. These equations are coupled to each other via exchange-correlation potentials which are universal functionals of the three densities. Approximations of these exchange-correlation functionals are derived using the diagrammatic techniques of many-body perturbation theory. The bare Coulomb repulsion between the electrons and the electron-phonon interaction enter this perturbative treatment on the same footing. In this way, a truly ab-initio description is achieved which does not contain any empirical parameters.

This new formalism is first applied to simple metals, to show the applicability to both weak and strong electron-phonon coupling. Further results for MgB_2, and Al and Li under pressure will be presented.