Density functional theory at finite temperature: Towards the ab-initio description of phase transitions

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Density functional theory (DFT) at finite temperature has the potential to describe phase transitions in an ab-initio way. How close to this goal we are with presently available approximate exchange-correlation functionals will be explored in this lecture. Two recent developments in finite-temperature DFT will be presented: In the first part, we develop a density functional formalism which describes superconductors at thermal equilibrium in terms of three quantities: the ordinary electronic density, the superconducting order parameter, and the nuclear N-body density. These three "densities" are determined self-consistently by a set of Kohn-Sham equations. The formalism can be viewed as the superconducting version of the multi-component density-functional theory for electrons and nuclei. Approximations of the universal exchange-correlation functional are derived on the basis of many-body perturbation theory. In this way, a true ab-initio description is achieved which does not contain any adjustable parameters such as the μ^* of Eliashberg theory. Numerical results for the critical temperature, the isotope effect, the gap function and the jump of the specific heat will be presented for simple metals, for MgB_2 , and for Li, Al, K and H under pressure. At the heart of finite-temperature DFT is the exchange-correlation part of the grand canonical potential which, in practice, needs to be approximated. Knowing the exact properties of this functional is essential to make good approximations. In the second part of the lecture, we will deduce exact features of this functional such as virial theorems and scaling laws. An interesting aspect in the formulation of scaling laws is that their formulation is possible only if the density and the temperature are scaled simultaneously.

Literature: