Public Abstract
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PhD
Physics
Theory of Lattice Effects on Magnetic Interactions in Solids
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The focus of this dissertation is the study of lattice oscillations on the magnetic properties of two families of materials. One class of materials is the $La_{1-x}Ca_xMnO_3$ series of manganites which exhibit colossal magneto-resistance in some regions of their phase diagram. The second consists of $Li_{1-x}Na_xNiO_2$ series of nickelate materials which may display unusual magnetic and orbital properties. Both these classes of materials have attracted considerable attention in recent years for their possible industrial applications, the manganites for their use as base materials for read heads in hard-drives and the nickelate as rechargeable battery storage materials.

This work is divided into five main parts: Introduction, Methods, EPC in a two-site system, Magnetism in $NaNiO_2$, and self-trapped magnetic polaron. Chapter 1 is the introduction to the dissertation, while Chapter 2 discusses the numerical and analytical methods used. In Chapter 3, the issue of the electron-lattice coupling is examined in a two-site model of the $LaMnO_3$, and the magnitude of the isotope effect on the critical temperature T_C is estimated. The electron-phonon coupling is shown to decrease the magnetic exchange from its Anderson-Hasegawa upper limit of $t\cos(\theta/2)$, and the oxygen isotope shift in T_C is estimated and found to agree well with experiments. Chapter 4 discusses the electronic structure and magnetism in $NaNiO_2$. The Variational Lang-Firsov method as well as exact diagonalization methods are used to show that inter-planar exchange is reduced by lattice coupling. The issue of different magnetic properties of $LiNiO_2$ compared to those of $NaNiO_2$ is discussed. Chapter 5 of the dissertation examines the magnetic polaron problem in a three dimensional lattice. The effect of the static Jahn-Teller coupling on the binding energy of the magnetic polaron is computed, as well as the effect of the next-nearest-neighbor hopping. The former is found to further stabilize the MP, while the latter has the opposite effect.