

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Sorting Category: 09.9.2 (C)

A realistic approach to effective Hamiltonians for strongly correlated electron materials: Study of orbital ordering in LaMnO₃¹

WEI-GUO YIN, DMITRI VOLJA, WEI KU, Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, Upton, NY 11973 — We present a general scheme to the realistic derivation of many-body effective Hamiltonians, H^{eff} , for strongly correlated electron systems: Based on a novel Wannier state analysis of the LDA+ U electronic structure, relevant mechanisms can be clearly singled out and their strengths can be accurately determined by mapping H^{eff} to the low-energy LDA+ U Hamiltonian within self-consistent Hartree-Fock mean-field theory [1]. Applying this scheme to LaMnO₃, the parent compound of colossal magnetoresistance manganites, we have quantified the relative importance of the effective electron-electron interaction (~ 1.7 eV) and the Jahn-Teller splitting (~ 0.9 eV) in ordering orbitals in LaMnO₃. We find that beyond the conventional Jahn-Teller picture, the electron-lattice (electron-electron) interaction alone is insufficient (sufficient) to stabilize the orbital ordering. Furthermore, our analysis indicates certain competition between different mechanisms, allowing direct experimental determination of their relative strengths. [1] W.-G. Yin, D. Volja, and W. Ku, cond-mat/0509075.

¹Work supported U.S. DOE.

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Prefer Oral Session
 Prefer Poster Session

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Date submitted: 06 Jan 2006

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