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Pseudo-spin of orbital-ordered hybridized e_g-states in manganites[1] WEI KU, WEI-GUO YIN, D. VOLJA, Physics Department, Brookhaven National Laboratory, Upton, NY 11973 — The physics of orbital-ordered e_g-states in manganites can be conveniently described with quantum pseudo-spin. In order to properly account for the strong hybridization in real materials, energy-resolved Wannier functions are constructed from first-principles to rigorously define the pseudo-spin in $LaMnO_3$ and MnF_3. Our quantitative results show that the orientation of the pseudo-spin (mixing of the hybridized e_g- states) deviates significantly from what is expected with the lattice distortion, revealing the important role of electron- electron interaction (super-exchange) that competes with the conventional Jahn-Teller effect in determining the orientation. This conclusion can be experimentally verified (*e.g.*: soft X- ray or NMR), and enables further understanding directly accessible with future measurements.

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