Spin-Orbit Interaction and the Jahn−Teller Effect

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In recent years, the effects associated with the spin-orbit interaction in various materials have been of great interest. These are topological insulators and semimetals, "Kitaev materials", spin-orbit Mott insulators, various compounds that can potentially be used in antiferromagnetic spintronics, etc. Despite close attention to the spin-orbit interaction, its effect on such a fundamental phenomenon as the Jahn–Teller effect has not been studied in depth. The development of numerical methods has made it possible to deal with this problem. We performed the exact diagonalization of the many-electron Hamiltonian containing the Coulomb, vibronic, and spin-orbit interactions in the case of t_{2g} electron orbitals (for e_g electrons, the orbital angular momentum is zero) and E and T phonons for all possible integer electron occupations. A nontrivial relation between the spin-orbit interaction, the Hund's rule intraatomic exchange, and the Jahn–Teller effect was revealed [1]. For example, for the d^1 configuration, the spin-orbit interaction suppresses the Jahn–Teller distortions, leading to a topology of the energy surface of the adiabatic potential of the Mexican hat type, which implies the existence of a Goldstone mode and can potentially be used for quantum computing. For the d^3 configuration, on the contrary, the spin-orbit interaction gives rise to Jahn–Teller distortions [2]. The results of such analysis are important for understanding the structural features of compounds based on heavy 4*d* and 5*d* transition metals and have been already used in the studies of physical properties of specific compounds.

[1] S. Streltsov and D. Khomskii, *Phys. Rev. X* **10**, 031043 (2020).
[2] S.V. Streltsov, F.V. Temnikov, K.I. Kugel, D.I. Khomskii, *Phys. Rev. B* **105**, 205142 (2022).