Quasi-static magnetoelectric quadrupoles as the order parameter for the pseudo-gap phase in cuprate superconductors

MICHAEL FECHNER, MERLIN J. A. FIERZ, FLORIAN THOLE, Materials Theory, ETH Zurich, Wolfgang-Pauli-Strasse 27, 8093 Zurich, URS STAUB, Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, NICOLA A. SPALDIN, Materials Theory, ETH Zurich, Wolfgang-Pauli-Strasse 27, 8093 Zurich — A characteristic of ferroic materials is the emergence of a temporally static finite expectation value of an order parameter. Here, we introduce a new mechanism [1] for ferroic order, in which a non-zero quasi-static magnetoelectric quadrupolar order appears due the coupling of fluctuating spin magnetic dipole moments and polar optical phonons. Using first-principles calculations within the LSDA+U method of density functional theory, we calculate the magnitude of the effect for the prototypical cuprate superconductor, HgBa$_2$CuO$_{4+\delta}$. We show that our proposed mechanism is consistent, to our knowledge, with many experimental observations for the onset of the pseudo-gap phase and therefore propose the quasi-static magnetoelectric quadrupole as a possible pseudo-gap order parameter. Finally, we show that our mechanism embraces some key aspects of previous theoretical models, in particular the description of the pseudo-gap phase in terms of orbital currents. [1] M. Fechner, M. J. A. Fierz, F. Thöle, U. Staub, and N. A. Spaldin, arXiv 1510.04844, (2015).