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Effect of electron-phonon interactions on orbital fluctuations in iron-based superconductors: a cDFPT study YUSUKE NOMURA, University of Tokyo, KAZUMA NAKAMURA, Kyushu Institute of Technology, RYOTARO ARITA, University of Tokyo — The pairing mechanism and symmetry of iron-based superconductors is still an open issue. So far, it has been shown that while spin-fluctuations mediate s-wave pairing with sign changes in the gap function ($s_{\pm}$-wave), orbital-fluctuations favor s-wave pairing without sign changes (s_{++}-wave). It has been recently proposed that electron-phonon (el-ph) interactions can enhance the orbital-fluctuations and thus contribute to the superconductivity. To examine the scenario quantitatively, it is highly important to derive, from first principles, an effective model including the phonon degrees of freedom. In this study, we develop an *ab initio* downfolding scheme for the el-ph coupled system, which we call constrained density-functional perturbation theory (cDFPT), and estimate the el-ph couplings and the phonon frequencies in the low-energy effective model for LaFeAsO [1]. We analyze the resulting model by the random phase approximation and show that, due to the small phonon-mediated effective exchange interaction, the $s_{\pm}$-wave instability is dominant. Therefore, we conclude that the el-ph interactions cannot be a driving force for the orbital-fluctuation-mediated s_{++}-wave state.

[1] Y. Nomura, K. Nakamura, R. Arita, arXiv:1305.2995

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