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Failure of the Holstein model to describe strong electron-phonon coupling[1] CLEMENS P.J. ADOLPHS, MONA BERCIU, Department of Physics and Astronomy, University of British Columbia, Vancouver, Canada — The coupling of electrons to phonons and the properties of the resulting quasiparticle, the polaron, are important for understanding many materials, including strongly correlated systems like the cuprates and the manganites. For some materials, the effective electron-phonon (el-ph) coupling λ is well known. For others, like the cuprates, estimates range from very small ($\lambda \sim 0.3$) to extremely large ($\lambda \sim 5$). Here, we point out an inconsistency in the widely used theoretical models. Both the Holstein and the Fröhlich model assume that lattice distortions are sufficiently small to allow treating the el-ph coupling as linear. At strong coupling, however, it is well established that a small polaron forms, with potentially considerable lattice distortions, invalidating the original assumption. We use the momentum average approximation to study the effect of higher-order coupling terms in the Holstein model. We show that they have drastic consequences on the properties of the polaron when compared to the linear model and that these effects cannot be captured by a linear model with renormalized parameters. Since linear models fail to describe strongly coupled systems, estimates of λ based on those models have to be reevaluated.

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