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Sharp transition for single polarons in one-dimensional models with non-diagonal Su-Schrieffer-Heeger coupling

DOMINIC J.J. MARCHAND, PHILIP C.E. STAMP, University of British Columbia, NIKOLAY V. PROKOF'EV, University of Massachusetts, MONA BERCIU, University of British Columbia — Ever since Landau pointed out the possibility of an electron becoming self-trapped in its own lattice distortion, people have looked for sharp transitions in polaronic states. Gerlach and Löwen [1] proved the absence of such a transition in the case of a gapped (i.e. optical) phonon branch and an electron-phonon coupling $g(q)$ depending only on the phonon momentum q . Whether a sharp transition could be found in other models remained an open question for the last twenty years. By presenting both unbiased Diagrammatic Monte Carlo results for the single polaron with Su-Schrieffer-Heeger (SSH) coupling to optical phonons, and supporting results from no less than three other numerical and analytical approximations, we believe our previous work and that of our collaborators [2] to be the first unequivocal demonstration of a sharp transition in a polaronic system. Here we expand this work to more general models that include either an additional diagonal Holstein coupling to optical phonons, or a SSH coupling to acoustic phonons. The survival of the sharp transition in these models is investigated using the Bold Diagrammatic Monte Carlo method and the Momentum Average approximation. References: [1] Rev. Mod. Phys. 63, 63 (1991) [2] Phys. Rev. Lett. 105, 266605 (2010)

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