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Bipolarons

in one-dimensional extended Peierls-Hubbard models¹ JOHN SOUS, Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia, Canada, V6T 1Z1, MONODEEP CHAKRABORTY, Indian Institute of Technology, Kharagpur, India, ROMAN KREMS, Department of Chemistry, University of British Columbia, Vancouver, British Columbia, Canada, V6T 1Z1, MONA BERCIU, Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia, Canada, V6T 1Z1 — We study two particles in an infinite chain and coupled to phonons by interactions that modulate their hopping as described by the Peierls/Su-Schrieffer-Heeger (SSH) model. In the case of hard-core bare particles, we show that exchange of phonons generates effective nearest-neighbor repulsion between particles and also gives rise to interactions that move the pair as a whole. The two-polaron phase diagram exhibits two sharp transitions, leading to light dimers at strong coupling and the flattening of the dimer dispersion at some critical values of the parameters. This dimer (quasi)self-trapping occurs at coupling strengths where single polarons are mobile. On the other hand, in the case of soft-core particles/ spinfull fermions, we show that phonon-mediated interactions are attractive and result in strongly bound and mobile bipolarons in a wide region of parameter space. This illustrates that, depending on the strength of the phonon-mediated interactions and statistics of bare particles, the coupling to phonons may completely suppress or strongly enhance quantum transport of correlated particles.

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