Abstract Submitted
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Efficient numerical technique for calculating the properties of interacting dimers in the Peierls-Hubbard model[1] JOHN SOUS, Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia, Canada, V6T 1Z1, MONODEEP CHAKRABORTY, Department of Physics, 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 develop a method to compute the Green's function for 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. The method is based on a variational approximation to the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY)ˆhierarchy and is shown to agree with exact digaonalization calculations. We show that the properties of bipolarons arising in such models is qualitatively different from those of the well-studied Holstein bipolarons. In particular, we show that depending on the particle statistics, strongly bound bipolarons may or may not form. In the case of hard-core bosons, we demonstrate novel effects for dimers such as sharp transitions and self-trapping. In the case of soft-core particles/ spinfull fermions, we show that the mediated interactions lead to overscreeing of the bare Hubbard U repulsion resulting in the formation of strongly bound bipolarons.

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