Abstract for GR-TR Conference on Statistical Mechanics and Dynamical Systems

Topic: Other Preference: Oral

Is there a barrier separating large and small polarons in one dimension?

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We discuss dimensionality effects of the Holstein polaron from the fully quantum regime, where the crossover between large and small polaron solutions is known to be continuous in all dimensions, into the limit described by the semiclassical Discrete Nonlinear Schrödinger (DNLS) Equation, where the crossover is continuous in 1D but discontinuous in higher dimensions. We use exact numerics on one hand and a two variable parametrization of the Toyozawa ansatz on the other in order to probe the crossover region in all parameter regimes. We show that a barrier appears also in 1D separating the two types of solutions, seemingly in contradiction to the common paradigm for the DNLS according to which the crossover is barrier-free. We quantify the polaron behavior in the crossover region as a function of the exciton overlap and find that the barrier remains small in 1D and tunnelling through it is not rate-limiting. We discuss ramifications of these findings in materials such as acetanilide.

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