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COMPUTATION OF NUMERICALLY EXACT STATIONARY AND MOVING POLAROBREATHERS

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In this work, we develop a numerical algorithm based on nonlinear least squares with constraints to obtain numerically exact stationary and moving polarobreather solutions [1], i.e., discrete breathers carrying charge, electron or hole, in semiclassical crystal lattice models. For the time integration of the nonseparable canonical Hamiltonian system, we consider a recently proposed structure-preserving numerical method that exactly preserves the total charge probability [2]. The essential properties of stationary and moving polarobreathers are deduced from the lattice and charge variables spectra in the frequency-momentum space, where the wave-characterization of exact discrete breathers has been put forward in [3; 4] in one and two-dimensional crystal lattice models, respectively. Authors in [1] have extended the wave theory to polarobreathers in semiclassical models. The spectrum of approximate polarobreather allows for determining the necessary parameters for the proposed numerical algorithm to compute exact polarobreathers, i.e., the fundamental time or period, the charge energy shift value, and the spatial step for moving solutions. The spectra of exact polarobreathers become extremely simple and easy to interpret. Understanding the polarobreather spectrum is fundamental to interpreting possible signatures of localized nonlinear waves in the physical spectra of real crystals. With our proposed methodology, we also solve the important problem that the charge frequency is not an observable, whereas the frequency of the charge probability, which is related to the discrete breather frequency, is an observable. Mathematical details of the methods, numerical results, and spectra of polarobreathers will be presented at the conference.

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