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Path-integral quantum Monte Carlo studies of lattice polarons and bipolarons PAVEL KORNILOVITCH, Hewlett-Packard Company, Corvallis OR — A path-integral Quantum Monte Carlo method for lattice polaron and bipolaron is presented. Analytical integration eliminates the phonons exactly leading to one or two self-interacting imaginary-time trajectories, which are then simulated by Metropolis Monte Carlo. Projection operators separate states of different symmetry, which provides access to various excited states such as the polaron energy, spectrum, effective mass, density of states and singlet-triplet bipolaron splitting. Monte Carlo updates are formulated in continuous imaginary time on infinite lattices and as such provide statistically unbiased results without finite-size and finite time-step errors. Numerical data are presented for models with short-range and long-range electron–phonon interactions. It is shown that a long-range electron-phonon interaction dramatically reduces the polaron and bipolaron mass, potentially leading to a high critical temperature of the bipolaronic superconductor.

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