Nonlinear impurity in a square lattice

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We use the Green?s-function formalism for an exact, numerical calculation of the stationary states of an electron propagating in a square lattice in the presence of a single, Holstein-type, impurity of arbitrary nonlinearity exponent. We find that two bound states exist above a certain exponent-dependent critical nonlinearity strength. The localization length of the lower (higher) energy bound state increases (decreases) with nonlinearity strength. The dynamics of an electron, initially placed on the impurity site, reveals a sharp, self-trapping transition for any nonzero nonlinearity exponent: below a certain nonlinearity threshold, the electron escapes from the impurity site ballistically; above the threshold, there is partial trapping at the impurity site while the untrapped fraction escapes to infinity, also ballistically. The self-trapping features are sharper in time and space than for its one-dimensional analogue. © 1999 The American Physical Society.