

Quantum vibrational impurity embedded in a one-dimensional chain

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We perform a fully quantum mechanical numerical calculation for the problem of a single electron (or excitation) propagating in an N -site one-dimensional chain in the presence of a single Holstein impurity. We compute the long-time averaged probability for finding the electron on the impurity site as a function of the nonlinearity parameter, defined in terms of the electron-phonon coupling strength and the oscillator frequency. The results, in the intermediate nonlinearity parameter range, differ substantially from the ones obtained through the use of the discrete nonlinear Schrödinger equation, even in the high-frequency regime. © 1997 Published by Elsevier Science B.V.