DYNAMICAL PROPERTIES OF DAVYDOV SOLITONS IN DISCRETE MOLECULAR CHAINS

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S u m m a r y

The dynamics of an autolocalized quasiparticle (electron, hole, vibrational or excitonic excitation) in a discrete lattice is investigated analytically and numerically, taking into account the quasiparticle interaction with longitudinal displacements of the molecules from their equilibrium positions (acoustic phonons). Such a system is described by the Fröhlich Hamiltonian and, in the continuum limit, supports the existence of Davydov solitons. It is shown that the correct account of the lattice discreteness results in a change of the dynamical properties of a Davydov soliton. Namely, it is shown that the dependence of the parameters of a soliton-like polaron on the carrying wave vector at large values of the latter differs from those predicted by the continuum models. It is proved numerically that the saturation of the soliton velocity in a discrete system occurs below the sound velocity in the chain, as is expected in the continuum model. This result is in agreement with the experimental observations of the saturation of the drift velocity of charge carriers in some low-dimensional compounds.

Numerous results of computer simulations of the soliton dynamics in molecular chains have demonstrated the existence of a potential barrier for the motion of a soliton from site to site. This potential is called the Peierls-Nabarro relief and is caused by the lattice discreteness. The value of this potential is calculated using the perturbation theory. Pinning of a soliton by such a barrier is studied numerically. It is shown that strongly localized, narrow solitons, close to a small-polaron state, can overcome the intersite barrier, provided their wave vector exceeds some critical value. This latter depends on the parameters of the chain and thus on the parameters of a soliton itself.