SELF-TRAPPING AND DYNAMICS OF A QUASI-PARTICLE IN A ONE-DIMENSIONAL MOLECULAR CHAIN UNDER INTERACTION WITH OPTICAL PHONONS

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S u m m a r y

The self-trapping conditions for a quasi-particle in a molecular chain are investigated taking into account the quasi-particle interaction with optical phonons, both dispersive and dispersionless. The dynamic properties of this soliton-like state of a quasi-particle are studied for various parameters of the model. The soliton velocity dependence on the wave vector is calculated and analyzed, and the soliton stability conditions are established. It is shown that the soliton velocity increases with the quasi-momentum to some saturation level. The soliton velocity is shown to be an oscillating function of the quasi-momentum, which is due to the Peierls—Nabarro barrier and the influence of optical phonons generated by the soliton. It is shown that the quasi-particle is self-trapped and dynamically stable for values of the wave vector less than the critical one. It is found that, for certain parameters corresponding to alpha-helical proteins, the quasi-particle can propagate over dozens of nanometers without considerable energy loss and without change of the envelope shape.