Localization of negative-effective-mass electron by supersonic kink in 1D lattice

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Abstract: Supersonic kink in nonlinear atomic chains with realistic interatomic potential produces local compression of the lattice. Lattice compression enhances electron Fermi energy and produces for an electron a local potential hill through the deformation potential of the proper sign. Such potential hill can localize (trap) negative-effective-mass (NEM) electron and such unconventional trapping can be observed in the simplest tight-binding model of electron band [1]. Here we confirm numerically the possibility of the trapping of NEM electron with the energy above the top of its tight-binding band by supersonic kink in the nonlinear lattices with two different interatomic potentials, the α-β FPU and Morse, and with the proper electron-phonon interaction. We reveal that the localization length of the electron wave function is much larger than lattice period in the case of adiabatic electron dynamics, electron localization length saturates for small-amplitude kink and continuously decreases with the increase of the velocity of the ultradiscrete supersonic kink. The ultradiscrete supersonic kinks, which were revealed in the nonlinear lattices with different interatomic potentials with hardening anharmonicity, have approximately sinusoidal envelope with the "magic" wave number [2,3]. The compression supersonic kink in the lattice with realistic asymmetric interatomic potential is accompanied by the local lattice expansion [2], which can trap positive-effective-mass electron.
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[1] Yu. A. Kosevich, Journal of Physics: Conf. Series **883**, 012021 (2017).
[2] Yu. A. Kosevich, Phys. Rev. Lett. **71**, 2058 (1993).
[3] Yu. A. Kosevich, R. Khomeriki, S. Ruffo, Europhys. Lett. **66**, 21 (2004).

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