

Contents

1	Introduction	1
	References	4
2	Acoustic Solitons	5
2.1	Fermi–Pasta–Ulam Problem (FPU)	5
2.2	Solitary Waves	11
2.3	Solitons in the Toda Chain	15
2.4	Numerical Methods for Finding Soliton Solution	18
2.5	Solitons in the Lennard-Jones Chain	19
2.6	Solitons in the Diatomic Chain	22
2.6.1	Model of the Diatomic Chain	22
2.6.2	Continuum Approximation	24
2.6.3	Numerical Simulation of Soliton Dynamics	24
2.7	Acoustic Solitons in a Helix Chain	26
2.7.1	Model of a Helix Chain	28
2.7.2	Dispersion Equation	31
2.7.3	Numerical Methods for Finding the Soliton Solution	34
2.7.4	Results of Numerical Analysis	40
2.7.5	Soliton Interaction	44
2.7.6	Modeling Acoustic Soliton Formation	45
2.7.7	Interaction of Solitons with Molecular Chain Heterogeneities	47
2.8	Conclusion	49
	References	49
3	Topological Solitons	53
3.1	Solitons in a Chain with Substrate	53
3.1.1	Stationary State of Topological Soliton	55
3.1.2	Interaction of Topological Solitons	58
3.1.3	Soliton Dynamics	60
3.1.4	Supersonic Regimes of Topological Soliton Motion	63

3.2	Solitons in an Anharmonic Chain	64
3.2.1	Stationary Soliton State	64
3.2.2	Vibrational Eigenmodes of a Topological Soliton.....	71
3.2.3	Numerical Method for Finding the Vibrational Eigenmodes	72
3.2.4	Vibrational Eigenmodes of a Soliton in the FPU- β Model ...	73
3.2.5	Vibrational Eigenmodes of a Kink in the FPU- α Model.....	75
3.2.6	Soliton Vibrational Eigenmodes in the Mixed FPU- α - β Model	76
3.2.7	Modeling Vibrational Eigenmodes.....	76
3.2.8	Supersonic Soliton Motion	79
3.2.9	Conclusion	90
3.3	Solitons in a Quasi-One-Dimensional Crystal.....	92
3.3.1	Modelling a Quasi-One-Dimensional Molecular System....	92
3.3.2	Immobile Neighbor Approximation	97
3.3.3	Dispersion of Low-Amplitude Waves	97
3.3.4	Stationary States of Topological Solitons	103
3.3.5	Topological Soliton Dynamics	107
3.3.6	Interaction of Topological Solitons	113
3.3.7	Formation of Topological Solitons in a Thermalized Lattice.....	117
3.3.8	Conclusion	118
	References	119
4	Localized Nonlinear Vibrations	123
4.1	A Nonlinear Oscillator	124
4.2	A Chain of Nonlinear Oscillators	126
4.3	Numerical Method for Finding Breathers.....	127
4.4	Properties of Discrete Breathers.....	128
	References	137
5	Ratchets	139
5.1	Asymmetric Pendulum	140
5.1.1	Potential Function of an Asymmetric Pendulum.....	141
5.1.2	Dynamical Equation	142
5.1.3	Asymmetry of Chaotic Oscillations.....	143
5.1.4	Asymmetric Particle Drift Velocity	144
5.1.5	Frequency Dependence of the Drift Velocity	145
5.1.6	Temperature Dependence of the Drift Velocity	145
5.1.7	Amplitude Dependence of the Drift Velocity.....	147
5.1.8	Isotope Dependence of the Particle Drift Velocity	148
5.1.9	Conclusion	148
5.2	Ratchet Dynamics of Solitons in the FK Model	149
5.2.1	Asymmetric Chain Model	150
5.2.2	Soliton Stationary State	151
5.2.3	Soliton Dynamics	156

5.2.4	Soliton Mobility	157
5.2.5	Soliton Motion Induced by Low-Frequency Noise	160
5.2.6	Conclusion	162
5.3	Numerical Simulation of Soliton Dynamics in the ϕ -4 Model	162
5.3.1	The Model.....	162
5.3.2	Asymmetry of Chain Monomer Oscillation	164
5.3.3	Stationary States of a Topological Soliton	166
5.3.4	Soliton Dynamics in a Thermalized Chain	168
5.3.5	Conclusion	169
	References	169
6	Solitons in Polymer Systems	171
6.1	Acoustic Solitons in Planar Zigzag PE Macromolecules and Spiral PTFE Macromolecules.....	172
6.1.1	Stretching Solitons PE Macromolecules.....	172
6.1.2	Stretching Solitons in a PTFE Macromolecule.....	181
6.2	Planar Solitary Waves in Graphite Layers and Soliton-Like Excitations in Carbon Nanotubes	194
6.2.1	Structure of Graphite Layers	194
6.2.2	Dispersion Equation of a Planar Wave in a Graphite Layer	197
6.2.3	Plane Solitary Waves in a Graphite Layer	199
6.2.4	Structure of a Carbon Nanotube	200
6.2.5	Dispersion Equation of Longitudinal Waves in Nanotube ...	202
6.2.6	Soliton-Like Excitations of Nanotubes	203
6.3	Topological Solitons in a Quasi-One-Dimensional Polymer Crystal	207
6.3.1	Topological Solitons in Crystalline PE	207
6.3.2	Topological Solitons in a Crystalline PTFE	224
6.4	Breathers in a PE Macromolecule	233
6.5	Conclusion	238
	References	239
7	Autolocalization of Quantum Particles	243
7.1	Davydov Soliton	249
7.1.1	General Dynamical Equations: Semi-classical Approximation	249
7.1.2	Soliton Dynamics in an Inhomogeneous Chain	252
7.2	Autolocalization of the Excitations in a β -Sheet	256
7.2.1	Discrete Model of Protein β -Sheet	256
7.2.2	Stationary States of Intrapeptide Excitation in β -Sheet Structures	259
7.2.3	Intrapeptide Excitation Dynamics in a β -Sheet	263
7.3	Soliton Dynamics of a Quasi-particle in an Anharmonic Chain	264
7.3.1	Acoustic Solitons	264
7.3.2	Numerical Method for Finding Acoustic Soliton Profile	267

7.3.3	Modeling the Dynamics of the Acoustic Soliton	268
7.3.4	Davydov Soliton and Bound States of a Quantum Quasi-particle with an Acoustic Soliton	271
7.3.5	Numerical Methods for Finding Quasi-particle Autolocalized States in an Anharmonic Chain	276
7.3.6	Two-Component Soliton Dynamics.....	280
7.3.7	Results of Numerical Investigation	282
7.4	Quasi-particle Autolocalization in a Chain with Substrate.....	285
7.5	Autolocalized State Dynamics of a Thermalized Chain.....	290
7.5.1	Acoustic and Optical Vibrations	291
7.5.2	Langevin Equation.....	292
7.5.3	Chain Thermalization.....	295
7.5.4	Soliton States of Intrapeptide Amide-I Excitation	299
7.5.5	Vibrational Lattice Model of the Amide-I Excitation Dynamics.....	303
7.5.6	Autolocalized State Dynamics of the Intrapeptide Amide-I Vibrations in a Thermalized Chain	304
7.6	Electrosoliton Dynamics in a Thermalized Chain	308
7.6.1	Estimation of Electron–Phonon Interaction Parameters	308
7.6.2	Model Hamiltonian	309
7.6.3	Stationary Autolocalized Electron States	311
7.6.4	Dynamics of Autolocalized Electron State in a Thermalized Chain	312
7.7	Resonant Effects of Microwaves Due to Their Interaction with Solitons in α -Helical Proteins	314
7.7.1	Biological Effects of EMR	314
7.7.2	Stationary Autolocalized States in Thermalized Molecular Chains	315
7.7.3	Stationary States of Excess Electrons in a Chain of PGs	318
7.7.4	Photodissociation of the Electrosoliton Under EMR.....	320
	References	323
	Index.....	331