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Concepts, Methods, and Applications

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With 161 Figures

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For Our Parents and Families

Preface

Theoretical physics deals with physical models. The main requirements for a good physical model are *simplicity* and *universality*. Universal models which can be applied to describe a variety of different phenomena are very rare in physics and, therefore, they are of key importance. Such models attract the special attention of researchers as they can be used to describe underlying physical concepts in a simple way. Such models appear again and again over the years and in various forms, thus extending their applicability and educational value. The simplest example of this kind is the model of a pendulum; this universal model serves as a paradigm which encompasses basic features of various physical systems, and appears in many problems of very different physical context.

Solids are usually described by complex models with many degrees of freedom and, therefore, the corresponding microscopic equations are rather complicated. However, over the years a relatively simple model, known these days as *the Frenkel-Kontorova model*, has become one of the fundamental and universal tools of low-dimensional nonlinear physics; this model describes a chain of classical particles coupled to their neighbors and subjected to a periodic on-site potential. Although links with the classical formulation are not often stated explicitly in different applications, many kinds of nonlinear models describing the dynamics of discrete nonlinear lattices are based, directly or indirectly, on a 1938 classical result of Frenkel and Kontorova, who applied a simple one-dimensional model for describing the structure and dynamics of a crystal lattice in the vicinity of a dislocation core. This is one of the first examples in solid-state physics when the dynamics of an extended defect in a bulk was modelled by a simple one-dimensional model. Over the years, similar ideas have been employed in many different physical problems, also providing a link with the mathematical theory of solitons developed later for the continuum analog of the Frenkel-Kontorova (FK) model.

In the continuum approximation, the FK model is known to reduce to *the exactly integrable sine-Gordon (SG) equation*, and this explains why the FK model has attracted much attention in nonlinear physics. The SG equation gives an example of a fundamental nonlinear model for which we know everything about the dynamics of nonlinear excitations, namely *phonons*, *kinks* (topological solitons), and *breathers* (dynamical solitons); and their multiparticle dynamics determines the global behavior of a nonlinear system as a whole. Although the FK model is inherently *discrete* and is not integrable, one may get a deep physical insight and simplify one's understanding of the nonlinear dynamics using the language of the SG nonlinear modes as weakly interacting effective quasi-particles. The discreteness of the FK model manifests itself in such phenomena as the existence of an effective periodic energy known as the Peierls-Nabarro potential.

The simplicity of the FK model, due to the assumptions of linear interatomic forces and a sinusoidal external potential, as well as its surprising richness and capability to describe a range of important nonlinear phenomena, has attracted a great deal of attention from physicists working in solid-state physics and nonlinear science. Many important physical phenomena, ranging from solitons to chaos as well as from the commensurate-incommensurate phases to glass-like behavior, present complicated sub-fields of physics each requiring a special book. However, the FK model provides a unique opportunity to combine many such concepts and analyze them together in a unified and consistent way.

The present book aims to describe, from a rather general point of view, *the basic concepts and methods of low-dimensional nonlinear physics* on the basis of the FK model and its generalizations. We are not restricted by the details of specific applications but, instead, try to present *a panoramic view* on the general properties and dynamics of solid-state models and summarize the results that involve fundamental physical concepts.

Chapter 1 makes an introduction into the classical FK model, while Chap. 2 discusses in more detail the applicability of the FK model to different types of physical systems. In Chap. 3 we introduce one of the most important concepts, the concept of kinks, and describe the characteristics of the kink motion in discrete chains, where kinks are affected by the Peierls-Nabarro periodic potential. In Chap. 4 we analyze another type of nonlinear mode, the spatially localized oscillating states often called *intrinsic localized modes* or *breathers*. We show that these nonlinear modes may be understood as a generalization of the SG breathers but exist in the case of strong discreteness. Chapters 3 and 4 also provide an overview of the dynamical properties of the generalized FK chains which take into account more general types of on-site potential as well as anharmonic interactions between particles in the chain. The effect of impurities on the dynamics of kinks as well as the dynamics and structure of nonlinear impurity modes are also discussed there. Chapter 5 gives a simple introduction to the physics of commensurate and incommensurate systems, and it discusses the structure of the ground state of the discrete FK chain. We show that the FK model provides probably the simplest approach for describing systems with two or more competing spatial periods. While the interaction between the atoms favors their equidistant separation with a period corresponding to the minimum of the interatomic potential, the interaction of atoms with the substrate potential (having its own period) tends to force the atoms into a configuration where they are regularly spaced. In Chap. 5 we employ two methods for describing the properties of the FK model: first, in the continuum approximation we describe the discrete model by the exactly integrable SG equation, and second, we study the equations for stationary configurations of the discrete FK model reducing it to the so-called *standard map*, one of the classical models of stochastic theory. The statistical mechanics of the FK model is discussed in Chap. 6, which also includes the basic results of the transfer-integral method. Here, the FK model again appears to be unique because, on the one hand, it allows the derivation of exact results in the one-dimensional case and, on the other hand, it allows for the introduction of weakly interacting quasi-particles (kinks and phonons) for describing the statistical mechanics of systems of strongly interacting particles. Chapter 7 gives an overview of the dynamical properties of the FK model at nonzero temperatures, including kink diffusion and mass transport in nonlinear discrete systems. Chapter 8 discusses the dynamics of nonlinear chains under the action of dc and ac forces when the system is far from its equilibrium state. Chapter 9 discuses ratchet dynamics in driven systems with broken spatial or temporal symmetry when a directed motion is induced. The properties of finite-length chains are discussed in Chap. 10, whereas two-dimensional generalizations of the FK model are introduced and described in Chap. 11, for both scalar and vector models. In the concluding Chap. 12 we present more examples where the basic concepts and physical effects, demonstrated above for simple versions of the FK chain, may find applications in a broader context. At last, the final chapter includes some interesting historical remarks written by *Prof. Alfred Seeger*, one of the pioneers in the study of the FK model and its applications.

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List of Abbreviations

CP	central peak
DW	double well (substrate potential); domain wall
DB	double barrier (substrate potential)
DSG	double sine-Gordon (equation)
FPK	Fokker-Planck-Kramers (equation)
FK	Frenkel-Kontorova (model)
FvdM	Frank – van der Merwe (limit)
GS	ground state
IC	incommensurate (phase)
LJ	Lennard-Jones (potential)
NS	nonsinusoidal (substrate potential)
SG	sine-Gordon (equation)
TI	transfer integral (method)
B	mobility
D	diffusion coefficient (D_k, D_η, D_a, D_s, D_μ, D_c)
E	(total) system energy
F	free energy; force
G	Gibbs free energy; Green's function
H	Hamiltonian
J	atomic flux
K	kinetic energy; transfer matrix; Chirikov's constant
L	length of a chain
M	number of wells of the substrate potential; memory function
N	number of atoms, kinks, breathers
P	kink momentum; misfit parameter
Q	correlation function; number of atoms in the cnoidal wave per period
R	distance between kinks
S	entropy
T	temperature; Chirikov map
U	total potential energy ($U_{\rm sub}$, $U_{\rm int}$)
V	potential energy ($V_{\rm sub}$, $V_{\rm int}$, V_{PN})
W	enthalpy
X	kink coordinate
Y	statistical sum $Y(T, \Pi, N)$; center of mass coordinate; point in the tour
Z	statistical sum $Z(T, L, N)$

a	lattice constant (a_s, a_A, $a_{\min}$, a_{FM})
c	sound speed
d	kink width
f	force; distribution function
g	elastic constant (g_{Aubry}, g_a, g_k)
h	discreteness parameter; hull function; scaling function
j	flux density
k	momentum; modulus (of elliptic function); wavevector
l	atomic index
m	kink mass
n	concentration of kinks (n_{tot}, n_k, n_w, n_{pair})
q	period of C-phase
r	used in window number, $w = r/s$
s	number of atoms in the unit cell, $\theta = s/q$; entropy per particle; spin
t	time
u	atomic displacement
v	kink velocity; interaction between kinks, v_{int}
w	displacement; window number, $w = r/s$
x	atomic coordinate
α	anharmonicity parameter
β	Boltzmann factor, $\beta \equiv (k_B T)^{-1}$
β	parameter for exponential interaction
γ	Lorentz factor; Euler constant
δ	phase shift (in collisions of kinks)
ε	energy (ε_s, ε_k, $\varepsilon_{\text{pair}}$, ε_{PN})
ψ	order parameter
κ	phonon momentum; parameter for Morse potential
χ	susceptibility; small displacement
λ	eigenvalues
ξ	correlation length; canonical variable
μ	chemical potential
η	friction coefficient; Bloch function
ρ	density (of atoms, phonons, kinks)
τ	dimensionless temperature, $\tau = k_B T/\varepsilon_k$
θ	dimensionless concentration (coverage), $\theta = N/M = s/q$
ω	frequency
$\omega_{\min}$	minimal phonon frequency of the pinned FK chain
σ	kink topological charge
ϵ	eigenvalues
Γ	phase volume
Δ	gap in spectrum
Π	pressure
Ξ	great statistical sum $\Xi(T, L, \mu)$
Ω	number of states; phase-space sharing; Mori function
Θ	step function
$\mathcal{N}$	response function
$\mathcal{L}$	Liouville operator
$\mathcal{P}$	projection operator

Table of Contents

1 Introduction

This introductory chapter is intended to provide a general overview of the classical formulation of the Frenkel-Kontorova model and its continuum version, the sine-Gordon equation. The chapter introduces also the fundamental modes of the model, phonons, kinks, and breathers, and describes some of their general properties. It also provides the background for the subsequent discussion of the basic physical systems where the nonlinear dynamics is described by the Frenkel-Kontorova model and its generalizations.

1.1 The Frenkel-Kontorova Model

A simple model that describes the dynamics of a chain of particles interacting with the nearest neighbors in the presence of an external periodic potential was firstly mentioned by Prandtl [1] and Dehlinger [2], see the historical notes of Prof. Alfred Seeger at the end of the book (see Chap. 13). This model was then independently introduced by Frenkel and Kontorova [3]–[6]. Such a chain of particles is presented schematically in Fig. 1.1. The corresponding mechanical model can be derived from the standard Hamiltonian,

$$\mathcal{H} = K + U, \tag{1.1}$$

where K and U are the kinetic and potential energies, respectively. The kinetic energy K is defined in a standard way,

$$K = \frac{m_a}{2} \sum_n \left(\frac{dx_n}{dt} \right)^2, \tag{1.2}$$

where m_a is the particle mass and x_n is the coordinate of the n-th particle in the chain. The potential energy U of the chain shown in Fig. 1.1 consists of two parts,

$$U = U_{\rm sub} + U_{\rm int}. \tag{1.3}$$

The first term $U_{\rm sub}$ characterizes the interaction of the chain with an external periodic on-site potential, taken in the simplest form,

$$U_{\rm sub} = \frac{\varepsilon_s}{2} \sum_n \left[1 - \cos\left(\frac{2\pi x_n}{a_s} \right) \right], \tag{1.4}$$