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Isaak A. Kunin

Elastic Media with Microstructure II

Three-Dimensional Models

With 20 Figures

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Professor *Isaak A. Kunin*

Department of Mechanical Engineering, University of Houston
Houston, TX 77004, USA

Guest Editor:

Professor Dr. Ekkehart Kröner

Institut für Physik, Universität Stuttgart
D-7000 Stuttgart 80, Fed. Rep. of Germany

Series Editors:

Professor Dr. Manuel Cardona
Professor Dr. Peter Fulde
Professor Dr. Hans-Joachim Queisser

Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1
D-7000 Stuttgart 80, Fed. Rep. of Germany

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Preface

Crystals and polycrystals, composites and polymers, grids and multibar systems can be considered as examples of media with microstructure. A characteristic feature of all such models is the existence of scale parameters which are connected with microgeometry or long-range interacting forces. As a result the corresponding theory must essentially be a nonlocal one.

This treatment provides a systematic investigation of the effects of microstructure, inner degrees of freedom and nonlocality in elastic media. The propagation of linear and nonlinear waves in dispersive media, static, deterministic and stochastic problems, and the theory of local defects and dislocations are considered in detail. Especial attention is paid to approximate models and limiting transitions to classical elasticity.

The book forms the second part of a revised and updated edition of the author's monograph published under the same title in Russian in 1975. The first part (Vol. 26 of Springer Series in Solid-State Sciences) presents a self-contained theory of one-dimensional models. The theory of three-dimensional models is considered in this volume.

I would like to thank E. Kröner and A. Seeger for supporting the idea of an English edition of my original Russian book. I am also grateful to E. Borie, H. Lotsch and H. Zorski who read the manuscript and offered many suggestions.

Houston, Texas
January, 1983

Isaak A. Kunin

Contents

1. Introduction

In recent years, new physical and mathematical models of material media, which can be considered far-reaching generalizations of classical theories of elasticity, plasticity, and ideal and viscous liquids, have been developed intensively. Such models have appeared for a number of reasons. Primary among them are the use of new construction materials in extreme conditions and the intensification of technological processes. The increasing tendency toward rapprochement of mechanics with physics is closely connected with these factors. The internal logic of the development of continuum mechanics as a science is also important.

This treatment is devoted to the study of models of elastic media with microstructure and to the development of the nonlocal theory of elasticity. Starting from such models as a crystal lattice and simple discrete mechanical systems, we develop the theory and its applications in a systematic way.

The Cosserat continuum was historically one of the first models of elastic media which could not be described within the scope of classical elasticity [1.1] However, the memoirs of *E.* and *F. Cosserat* (1909) remained unnoticed for a long time, and only around 1960 did the generalized models of the Cosserat continuum start to be developed intensively. They are known as oriented media, asymmetric, multipolar, micromorphic, couple-stress, etc., theories. For short we shall call them couple-stress theories. Essential contributions to the development of couple-stress theories were made, for example, by Aero, Eringen, Green, Grioli, Günther, Herrmann, Koiter, Kuvshinsky, Mindlin, Naghdi, Nowacki, Palmov, Rivlin, Sternberg, Toupin, and Wozniak; their fundamental works are listed in the Bibliography. The Bibliography is far from being complete. A survey of works before 1960 can be found in the fundamental treatment of *Truesdell* and *Toupin* [1.2]; later ones are quoted in papers by *Wozniak* [1.3], *Savin* and *Nemish* [1.4], *Iliushin* and *Lomakin* [1.5], as well as in monographs by *Misicu* [1.6] and *Nowacki* [1.7].

From the very beginning of the development of the generalized Cosserat models, attention was turned to their connections with the continuum theory of dislocations. In 1967 a symposium was organized by the International Union of Theoretical and Applied Mechanics, which had great significance in summing up the ten-year period of development [1.8]. In the symposium a new trend closely connected with the theory of the crystal lattice was also presented which contained the above-indicated models as a long-wave approximation, namely, a nonlocal theory of elasticity. The nonlocal theory of elasticity was also developed in works of Edelen, Eringen, Green, Kröner, Kunin, Laws and others, given in the Bibliography. A rather complete listing on media with microstructure is contained in [1.9]. It is worth mentioning here that the very term "nonlocal elasticy" seems to have been introduced by *Kröner* in 1963 [1.10], and the first monograph on the subject was published by the present author in 1975 [1.11].

We start out with a brief classification of the theories of elastic media with microstructure. Explicit or implicit nonlocality is the characteristic feature of all such theories. The latter, in its turn, displays itself in that the theories contain parameters which have the dimension of length. These scale parameters can have different physcial meanings: a distance between particles in discrete structures, the dimension of a grain or a cell, a characteristic radius of correlation or action-at-a-distance forces, etc. However, we shall always assume that the scale parameters are small in comparison with dimensions of the body.

One has to distinguish the cases of strong and weak nonlocality. If the "resolving power" of the model has the order of the scale parameter, i.e., if, in the corresponding theory, it is physically acceptable to consider wavelengths comparable with the scale parameter, then we shall call the theory nonlocal or strongly nonlocal (when intending to emphasize this). In such models, one can consider elements of the medium of the order of the scale parameter, but, as a rule, distances much smaller than the parameter have no physcial meaning. The equations of motion of a consistently nonlocal theory necessarily contain integral, integrodifferential, or finite-difference operators in the spatial variables. In nonlocal models, the velocity of wave propagation depends on wavelength; therefore, the term "medium with spatial dispersion" is also used frequently.

Let us emphasize that nonlocality or spatial dispersion can have different origins. They can be caused by a microstructure of the medium (in particular, by the discreteness of the micromodel) or by approximate consideration of such parameters as thickness of a rod or plate. One can speak therefore about the physical or geometrical nature of nonlocality. In the latter case, the nonlocal model is, as a rule, one- or two-dimensional and serves as an effective approximate description of a local three-dimensional medium.

If the scale parameter is small in comparison with the wavelengths considered, but the effects of nonlocality cannot be neglected completely, then a transition is possible to approximate models, for which integral and finite-difference operators are replaced by differential operators with small parameters attached to their highest derivatives. In such a case, one can speak about the model of the medium with weak spatial dispersion. The corresponding theory will be called weakly nonlocal. All above-mentioned couple-stress theories belong to this type, although they are usually constructed on a purely phenomenological basis.

Finally, the consideration of sufficiently long waves (zeroth long-wave approximation) leads to a transition to a local theory in the limit, already containing no scale parameters. This property of locality, i.e., the possibility of considering "infinitesimally small" elements of the medium, is inherent in all the classical models of the mechanics of continuous media.

Let us return to nonlocal models. They can be divided into two classes: discrete and continuous. Discrete structure of a medium could be taken into account in the usual way, for example, as is done in the theory of the crystal lattice. However, the apparatus of discrete mathematics is most cumbersome; therefore, we shall also use the mathematical model of quasicontinuum for an adequate description of the discrete medium. Its essence is an interpolation of functions of discrete argument by a special class of analytical functions in such a way that the condition of one-to-one correspondence between quasicontinuum and the discrete medium is fulfilled. The advantages of such an approach consist in an ability to describe discrete and continuous media within the scope of a unified formalism and, in particular, to generalize correctly such concepts of continuum mechanics as strain and stress. It is to be emphasized that the model of quasicontinuum is applicable not only to crystal lattices but also to macrosystems.

We shall also distinguish media of simple and complex structures. In the first case, the displacement vector is the only kinematic variable and it determines a state of the medium completely. Body forces are the corresponding force variable. To describe a medium of complex structure, a set of microrotations and microdeformations of different orders characterizing the internal degrees of freedom and the corresponding force micromoments is additionally introduced.

The difference between media of simple and complex structures, generally speaking, is conserved in the approximation of weak nonlocality, but this is displayed only for high enough frequencies of the order of the natural frequencies of the internal degrees of freedom. At low frequencies, the internal degrees of freedom can be excluded from the equations of motion so that they will contribute to the effective characteristics of the medium only. The difference between the quasicontinuum and the continuous medium completely disappears in the approximation of weak nonlocality.

In the zeroth long-wave approximation, at not very high frequencies, a complete identification of different models of a medium with microstructure takes place: all of them are equivalent to the classical model of elastic continua which was obtained on the basis of general phenomenological postulates. Only effective elastic moduli "know" about the structure of the initial micromodel, but this information cannot, of course, be derived from them. It follows that an explicit consideration of microstructure effects and, in particular, of the internal degrees of freedom is possible only with the simultaneous consideration of nonlocality, i.e., a consistent theory of elastic medium with microstructure must necessarily be nonlocal.

Schematically, the connections between different theories are shown in Fig. 1.1.

Our main purpose is the investigation of the effects of microstructure and nonlocality. In addition, we wish to elucidate the domain of applicability of different theories of media with microstructure. Such theories are considerably more complex than the usual theory of elasticity, although they reduce to this in

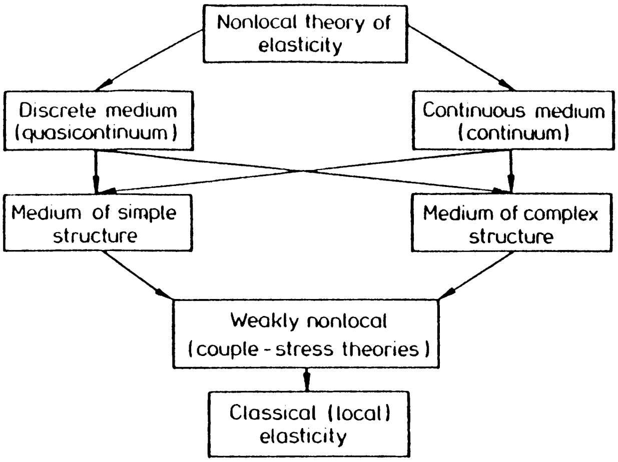

Fig. 1.1. Illustrating the interconnections of the various theories

certain limits; their application is, as a rule, reasonable only when they describe qualitatively new effects which are not derivable from the local theory.

We find it advisable to consider a number of simple models of media with microstructure in order to acquire some nonlocal intuition before proceeding to generalizations.

For these reasons, the treatment is divided into two parts. One-dimensional models, for which cumbersome tensor algebra is not needed, are studied in the first volume [1.12]. At the same time, one can trace a number of distinctions of the nonlocal theory from the local one already in one-dimensional models. These distinctions have both physical and methodological character. Particularly, one has to analyze critically the possibility of using in nonlocal theories such habitual notions as stress, strain, energy, density and flux.

In this volume, three-dimensional models of media with microstructure are considered, the main attention being payed to specific three-dimensional effects. The second and third chapters are devoted to the general theory of media with simple and complex structures. Local defects in media with microstructure as well as in elasticity are considered in Chapter 4. Internal stress and dislocations in the nonlocal elasticity are considered in Chapters 5 and 6. Chapter 7 (written by S.K. Kanaun) is devoted to random fields of inhomogeneities.

The author has tried to avoid complex mathematical methods in the first part. It is assumed that the reader is acquainted with the Fourier transform and has some skill in working with δ-functions (though it is easy to acquire it in the process of reading the book).

The necessity of simultaneous use of space-time and frequency-wave representations is one of the peculiarities of the formalism used in the nonlocal theory. This way of thinking is quite habitual for physicists, but could be, to some extent, unusual for engineers. Because of this, the rate of presenting the material is slow in the beginning and then speeds up gradually. For the same purpose, a number of results are presented in the form of problems, which are considered a part of the text and they are referred to in the later text.

In conclusion, let us note that a number of important questions are omitted. In particular, this is related to the thermodynamics of the nonlocal models, which was contained in the original plan of the book. Unfortunately, the author has not succeeded in representing this problem in a sufficiently simple and physically motivated form. An axiomatic approach to the nonlocal thermodynamics was developed by *Edelen* [1.13].

2. Medium of Simple Structure

In this chapter, we consider in detail the three-dimensional elastic medium of simple structure. To describe, in the same language, discrete and continuum non-local models, we introduce the three-dimensional quasicontinuum. Then, starting from crystal dynamics, we obtain the general nonlocal equations of motion for the medium of simple structure. We investigate the consequences of such physical requirements as energy conservation, finite action-at-a-distance, stability and invariance of the energy with respect to rigid body motions. In particular, the last requirement leads to the existence of a symmetric stress tensor. In contrast to the local elasticity, the stress and energy density are not defined uniquely in nonlocal elasticity.

The second part of the chapter is devoted to homogeneous media. Wave propagation (including surface waves) in dispersive media and the corresponding physical phemomena are examined. Approximate theories that can describe partially these effects are discussed. As examples of nonlocal media, a cubic lattice and isotropic models are considered.

2.1 Quasicontinuum

Let us suppose that in a three-dimensional Euclidean space E_3 with points x, a triple of noncoplanar vectors $e_\alpha(\alpha = 1, 2, 3)$ with a common origin at the point x_0 is given. The set of points in E_3, which is obtained through all displacements of the origin by vectors[1] $n^\alpha e_\alpha(n$ and α being aribtrary integers) forms a (simple) lattice with an elementary cell of the form of parallelepiped, constructed on e_α. Points of this lattice are also called knots.

It is convenient to introduce oblique lattice coordinates x^α with the origin at the point x_0, basis vectors e_α and a metric tensor $g_{\alpha\beta}$, which is equal to the scalar product of the basis vectors: $g_{\alpha\beta} = (e_\alpha, e_\beta)$. Then, to knots of a lattice there correspond combinations of vectors $n = n^\alpha e_\alpha$ with integer components n^α.

Let $u(n)$ be a scalar or tensor, generally a complexvalued function, which is given at knots and which increases no faster than a power of $|n|$ as $|n| \to \infty$. Then analogously to the one-dimensional case [1.12], the function $u(n)$ can be interpolated by a generalized analytic function $u(x)$, which is uniquely deter-

[1]Here and in the following material by identical superscripts and subscripts we contemplate summation.

mined by some natural conditions. In order to avoid repetition, we shall concentrate on the special features of the three-dimensional case in the following.

Together with the interpolating function $u(x)$ let us also consider its Fourier transform:

$$u(k) = \int u(x)\mathrm{e}^{-\mathrm{i}kx}\,dx\,. \tag{2.1.1}$$

Here, kx is, strictly speaking, a linear function, which is conveniently written in the form of a scalar product. As is well-known, the space E_3 of all linear functions of x is a three-dimensional vector space (k-space), where the basis e^β is introduced; it is reciprocal to the basis e_α:

$$e^\beta e_\alpha = e^\beta(e_\alpha) = \delta^\beta_\alpha\,. \tag{2.1.2}$$

Then $k = k_\beta e^\beta$ and $kx = k_\alpha x^\alpha$. Note that the last expression is also understood as an ordinary scalar product (k, x), if between the spaces E_3 (with fixed origin) and E_3' an identification is established with the help of the metric tensor $g_{\alpha\beta}$, i.e., the operation of raising and lowering of indices. For our purpose such an identification is not convenient and we shall consider separately the "physical" x-space E_3 and the dual k-space E_3'.

Let us construct a parallelepiped $\mathrm{B}\{-\pi \le k_\beta \le \pi\}$, in the k-space, whose edges are parallel to vectors of the reciprocal basis e^β and set

$$\delta_\mathrm{B}(x) \overset{\mathrm{def}}{=} \frac{1}{(2\pi)^3}\int_\mathrm{B} \mathrm{e}^{\mathrm{i}xk}\,dk = \frac{1}{\pi^3 v_0}\prod_{\beta=1}^{3}\frac{\sin(xe^\beta)}{xe^\beta}\,, \tag{2.1.3}$$

where v_0 is the volume of an elementary cell constructed on the vectors e_α. It is obvious that $\delta_\mathrm{B}(0) = v_0^{-1}$ and $\delta_\mathrm{B}(n) = 0$ for all other knots.

Let us assume that $u(n)$ decreases sufficiently rapidly as $|n| \to \infty$. Then in B one can define a function $u(k)$, such that the coefficients of its Fourier series are equal to $v_0 u(n)$, i.e.

$$u(k) = v_0 \sum_n u(n)\mathrm{e}^{\mathrm{i}nk}, \qquad k \in \mathrm{B}\,. \tag{2.1.4}$$

Defining $u(k)$ to be zero outside B, and taking into account (2.1.3) we find for the inverse Fourier transform $u(x)$

$$u(x) = v_0 \sum_n u(n)\delta_\mathrm{B}(x - n)\,. \tag{2.1.5}$$

It is possible to prove that the function $u(x)$ can be continued analytically into the complex plane as an entire function of exponential type $\le \pi$.

In view of the properties of $\delta_\mathrm{B}(x)$, it is easy to see that $u(x)$, defined by (2.1.5), is in fact the required interpolating function. The one-to-one correspondence

$u(n) \leftrightarrow u(x) \leftrightarrow u(k)$ is well guaranteed by the condition of truncating the Fourier-transform $u(k)$ of the function $u(x)$ and the uniqueness of the expansion (2.1.4).

Let us proceed to the general case of the space $N'(\mathrm{B})$, whose elements are functions $u(n)$, which increase no faster than some power of $|n|$ as $|n| \to \infty$. The space $N'(\mathrm{B})$ can also be regarded as a space of generalized functions on the space $N(\mathrm{B})$, the latter being the space of rapidly decreasing functions.

Recall that in the one-dimensional case [1.12], when interpolating functions $u(n) \in N'(\mathrm{B})$, it turned out to be necessary to identify the ends of the segment B, transforming it into a circle. Analogously, let us identify the opposite faces of the present parallelepiped B or, in other words, let us transform it into a three-dimensional torus.

The series (2.1.4) now converges only in the sense of the generalized functions [2.1], and $u(k)$ belongs to the space of the generalized functions $K'(\mathrm{B})$, defined on the space $K(\mathrm{B})$ of infinitely differentiable test functions with supports in B.

Let us denote the inverse Fourier transforms of the spaces $K(\mathrm{B})$ and $K'(\mathrm{B})$ by $X(\mathrm{B})$ and $X'(\mathrm{B})$, respectively. The inverse Fourier transform $u(x) \in X'(\mathrm{B})$ of a function $u(k) \in K'(\mathrm{B})$ is defined, as usual, with the help of the Parseval equality

$$\int \overline{u(x)}\varphi(x)dx = \frac{1}{(2\pi)^3} \int \overline{u(k)}\varphi(k)dk\,, \tag{2.1.6}$$

where $\varphi(x) \in X(\mathrm{B})$ and $\varphi(k) \in K(\mathrm{B})$ are connected with each other by the usual Fourier transform.

It can be proved [2.1] that $u(x) \in X'(\mathrm{B})$ are regular generalized functions (i.e. corresponding to ordinary functions), which increase no faster than a power of $|x|$ as $|x| \to \infty$ and which can be analytically continued to a complex region as entire functions of the exponential type $\leq \pi$. The proof of the fact that the function $u(x)$ has values $u(n)$ at the knots, can be performed analogously to the one-dimensional case [1.12].

The uniqueness of interpolation is ensured by the identification of the opposite faces of the parallelepiped B. This excludes from $X'(\mathrm{B})$ functions of the type $P(x)\sin[\pi(xe)^\beta]$, [$P(x)$ being a polynomial], which vanish at all the knots.

Thus we have:

Theorem. The formulae (2.1.4, 6) fix linear isomorphisms between the spaces

$$N'(\mathrm{B}) \leftrightarrow X'(\mathrm{B}) \leftrightarrow K'(\mathrm{B})\,, \tag{2.1.7}$$

such that $u(x) \in X'(\mathrm{B})$ interpolates $u(n) \in N'(\mathrm{B})$.

We may now consider $u(n)$, $u(x)$ and $u(k)$ as representations of one and the same function in different functional bases. Of course, to this end it is also necessary to know the corresponding representations of operations over these functions.

A function $q(n)$, which decreases rapidly, as $|n| \to \infty$ (in particular, a function with finite support), determines the linear functional

$$\langle q|u\rangle \stackrel{\text{def}}{=} \sum_n \overline{q(n)}u(n) = \int \overline{q(x)}u(x)dx = \frac{1}{(2\pi)^3}\int \overline{q(k)}u(k)dk\,, \tag{2.1.8}$$

which is invariant with respect to the $n-$, $x-$, and k-representations, if the kernels $q(n)$, $q(x)$ and $q(k)$ are connected by the relations

$$q(k) = \sum_n q(n)e^{-ink}, \qquad k \in \mathrm{B}\,,$$
$$q(x) = \sum_n q(n)\delta_{\mathrm{B}}(x - n)\,. \tag{2.1.9}$$

Problem 2.1.1. Prove the above proposition.

Note that, as distinct from (2.1.4, 5), in the correspondence $q(n) \leftrightarrow q(x) \leftrightarrow q(x)$ the factor v_0 is absent. This is connected with the fact that in the further consideration the quantities $q(n)$ will have the meaning of forces acting at the knots of a lattice. Thus $q(x)$ can be interpreted as the corresponding density of body forces, $q(k)$ as its Fourier transform and the functional $\langle q|u\rangle$ as the work, done by the forces q on the displacement u.

As an important example, consider the functional

$$\langle \delta|u\rangle = u(n)\,|_{n=0} = u(x)\,|_{x=0} = \int_{\mathrm{B}} u(k)dk \tag{2.1.10}$$

with the kernels

$$\delta(n) \leftrightarrow \delta_{\mathrm{B}}(x) \leftrightarrow 1(k)\,. \tag{2.1.11}$$

Here $\delta(n) = 1$ at $n = 0$, and it is equal to zero at all other knots. Evidently, $\delta_{\mathrm{B}}(x)$ plays in $X'(\mathrm{B})$ the role of an ordinary δ-function but, as distinct from the latter $\delta_{\mathrm{B}}(x)$ is not singular. In what follows, we shall use the notation $\delta(x)$ instead of $\delta_{\mathrm{B}}(x)$ when this does not lead to any misunderstandings.

Problem 2.1.2. Show that the following identities are generated by the functional with the kernel $1(x)$:

$$v_0 \sum u(n) = \int u(x)dx = u(k)\,|_{k=0}\,. \tag{2.1.12}$$

Analogously to the one-dimensional case [1.12] we define the invariant form

$$\langle u|\Phi|w\rangle \overset{\text{def}}{=} \sum_{nn'} \overline{u(n)}\Phi(n, n')w(n') = \iint \overline{u(x)}\Phi(x, x')w(x')dx\, dx'$$

$$= \frac{1}{(2\pi)^3}\iint \overline{u(k)}\Phi(k, k')w(k')dk\ dk' = \overline{\langle w|\Phi^+|u\rangle}\,. \tag{2.1.13}$$

Here

$$\Phi(k, k') = \frac{1}{(2\pi)^3}\sum_{nn'}\Phi(n, n')\mathrm{e}^{-\mathrm{i}(kn-k'n')}$$

$$= \frac{1}{(2\pi)^3}\iint \Phi(x, x')\mathrm{e}^{-\mathrm{i}(kx-k'x')}dx\, dx'\,, \tag{2.1.14}$$

$$\Phi^+(k, k') = \overline{\Phi(k',k)}, \qquad \Phi^+(x, x') = \overline{\Phi(x', x)}\,. \tag{2.1.15}$$

One can establish the correspondences between the discrete and continuous operations of multiplication, convolution, differentiation and so on, distinctions compared with the one-dimensional case being small.

Thus, the functions $u(n) \in N'(\mathrm{B})$ constitute a ring with respect to the operation of multiplication. At the same time, the ordinary product of two functions from $X'(\mathrm{B})$, generally speaking, does not belong to $X'(\mathrm{B})$. Nevertheless, it is possible to introduce in $X'(\mathrm{B})$ such an operation of multiplication, which corresponds to the multiplication of the inverse transforms in $N'(\mathrm{B})$ and whose result is still contained in $X'(\mathrm{B})$.

In fact, on the torus B we can define an operation of displacement and, hence, an integral convolution

$$u(k) * w(k) = \int_{\mathrm{B}} u(k - k')w(k')dk', \tag{2.1.16}$$

with respect to which $K'(\mathrm{B})$ is a ring.

Problem 2.1.3. Verify the correspondence

$$f(n) = u(n)w(n) \leftrightarrow f(k) = u(k) * w(k)\,. \tag{2.1.17}$$

This leads to the natural definition of the product, in $X'(\mathrm{B})$:

$$f(x) = u(x)\cdot w(x) \leftrightarrow f(k) = u(k) * w(k)\,. \tag{2.1.18}$$

Problem 2.1.4. Show that $f(x)$ coincides with $f(n)$ at all knotes.

In particular, the following formulae are valid:

$$u(x)\delta(x) = u(0)\delta(x), \ \delta(x)\delta(x) = v_0\delta(x)\,. \tag{2.1.19}$$

Here, we observe from a new point of view, the expedience of transforming the parrallelepiped B into a torus, since it is impossible to find a reasonable definition of a convolution on a parallelepiped such that the support of $u(k)*w(k)$ is always contained in the parallelepiped.

Note that if the supports of $u(k)$, $w(k) \in K'(\mathrm{B})$ are contained in a parallelepied similar to B, but twice smaller, then, the convolution in (2.1.16) coincides with the ordinary one and hence the above-defined multiplication also coincides with the ordinary one. Of course, this will also happen if one of the factors is a polynomial (in the x-representation), since its support (in the k-representation) is concentrated at the point $k = 0$.

The algorithm considered above for passing from functions of discrete argument to functions of continuous argument may be clearly interpreted as spanning some analytic structure over the lattice in such a way that one-to-one correspondence between the structures is conserved. The Euclidean space in which only functions from $X'(\mathrm{B})$ are allowed, is conveniently interpreted as a quasicontinuum, its geometry being isomorphic to that of a lattice. When the size of elementary cell of the lattice tends to zero (this is equivalent to the consideration of functions which change only slightly over distances of the order of the cell size), the region B extends over all k-space and the quasicontinuum is transformed into a continuum with the ordinary geometry.

The idea of quasicontinuum can be naturally generalized by taking, instead of the parallelepiped B, another manifold. The isotropic continuum will be of considerable importance, the corresponding region B being a sphere. The replacement of the parallelepiped by a sphere in k-space was first carried out by Debye in order to calculate the heat capacity of a crystal and was further widely used for qualitative estimates of physical properties of crystals (without any connection with the idea of the quasicontinuum). The radius κ of the sphere is usually determined by the condition of equality of the volumes of the sphere and the parallelepiped. The exact correspondence with the lattice structure is lost in this case, but the corresponding quasicontinuum model, which will be called the Debye model, describes qualitatively correctly the presence of a discrete structure with the characteristic scale parameter $a \simeq \pi/\kappa$.

The Debye model can be somewhat improved by identifying the opposite points of the boundary sphere analogously to identifying opposite faces of the parallelepiped. In this case, the manifold B, will be homeomorphic to a three-dimensional projective space.

As another example we can mention a layered medium, in which the characteristic scale parameter is to be introduced in one direction only. Accordingly, in the k-space, transform is to be carried out with respect to one coordinate only.

In the general case, the quasicontinuum of class B may be defined as the set of two objects: an Euclidean space and a space of admissible functions $X'(\mathrm{B})$ given on that space, B being a fixed manifold.

2.2 Equations of Motion

The model for a medium with simple structure will be based on Born's model of a simple lattice with the basis e_α in the harmonic approximation. For the elastic energy Φ we have, analogously to the case of a one-dimensional chain [1.12],

$$\Phi = \frac{1}{2} \sum_{nn'} u_\alpha(n)\, \Phi^{\alpha\beta}(n, n') u_\beta(n') , \tag{2.2.1}$$

where $\Phi^{\alpha\beta}(n, n')$ is a given tensor of the force constants, and $u_\alpha(n)$ is the displacement of the particles from the equilibrium position, i.e. it is assumed that initial external forces are absent.

This model may be interpreted, if necessary, as a system of pointwise particles situated at the knots of the lattice and interacting by means of linear elastic bonds of the most gêneral nature.

The Lagrangian of this system has the form

$$L = \frac{1}{2} g^{\alpha\beta} \sum_n m(n)\dot{u}_\alpha(n)\dot{u}_\beta(n) - \frac{1}{2} \sum_{nn'} u_\alpha(n)\Phi^{\alpha\beta}(n, n')u_\beta(n') - \sum_n q^\alpha(n)u_\alpha(n) , \tag{2.2.2}$$

where $m(n)$ is the mass of a particle at the point n, and $q^\alpha(n)$ is the external force acting on the particle. The dependence of the field parameters on time is not indicated explicitly.

In the usual way we find the equations of motion

$$m(n)\ddot{u}^\alpha(n) + \sum_{n'} \Phi^{\alpha\beta}(n, n')u_\beta(n') = q^\alpha(n) . \tag{2.2.3}$$

Using the above-described algorithm, let us proceed to a quasicontinuum representation. For the elastic energy Φ we have, cf. (2.1.13)

$$\Phi = \frac{1}{2} \langle u_\alpha|\Phi^{\alpha\beta}|u_\beta\rangle = \frac{1}{2} \iint u_\alpha(x)\Phi^{\alpha\beta}(x, x')\, u_\beta(x')dx\, dx' = \frac{1}{(2\pi)^3} \iint \overline{u_\alpha(k)}\Phi^{\alpha\beta}(k, k')u_\beta(k')dk\, dk' , \tag{2.2.4}$$

where $\Phi^{\alpha\beta}(x, x')$ and $\Phi^{\alpha\beta}(k, k')$ are expressed in terms of the force constants

$$\Phi^{\alpha\beta}(k, k') = \frac{1}{(2\pi)^3} \sum_{nn'} \Phi^{\alpha\beta}(n, n')e^{-i(kn-k'n')} = \frac{1}{(2\pi)^3} \iint \Phi^{\alpha\beta}(x, x')e^{-i(kx-k'x')}\, dx\, dx' . \tag{2.2.5}$$

Introducing the mass density $\rho(x)$ and force density $q(x)$

$$\rho(x) = \sum_n m(n)\delta(x - n), \quad q(x) = \sum_n q(n)\delta(x - n), \tag{2.2.6}$$

we write the Lagrangian (2.2.2) in the form

$$L = \frac{1}{2}\langle \dot{u}_\alpha|\rho g^{\alpha\beta}|\dot{u}_\beta\rangle - \frac{1}{2}\langle u_\alpha|\Phi^{\alpha\beta}|u_\beta\rangle + \langle q^\alpha|u_\alpha\rangle, \tag{2.2.7}$$

where the operator ρ has the kernel $\rho(x)\delta(x - x')$.

If we do not assume the existence of a discrete micromodel, then the Lagrangian in the form or (2.2.7) corresponds to the most general nonlocal theory of an elastic medium with simple structure. In this case, the admissible functions are not restricted by truncation of their Fourier transforms, i.e., all the field quantities are considered to be given on an ordinary manifold. The quasicontinuum (discrete) model is, in fact, a particular case of the general theory.

The equations of motion, which correspond to the Lagrangian (2.2.7) have the form

$$\rho(x)\ddot{u}^\alpha(x) + \int \Phi^{\alpha\beta}(x, x')u_\beta(x')dx' = q^\alpha(x), \tag{2.2.8}$$

$$(2\pi)^{-3}\rho(k) * \ddot{u}^\alpha(k) + \int \Phi^{\alpha\beta}(k, k')u_\beta(k')dk' = q^\alpha(k) \tag{2.2.9}$$

in the x- and k-representations, respectively. In the case of the quasicontinuum, the n-representation (2.2.3) is to be added.

The equations of motion are conveniently considered in the ω-representation. In operator form, they have the form cf. (2.1.37),

$$(-\rho\omega^2\delta^{\alpha\beta} + \Phi^{\alpha\beta})u_\beta = q^\alpha. \tag{2.2.10}$$

Obviously, the physical content of the equations of motion is determined, first of all, by properties of the operator of the elastic energy $\Phi^{\alpha\beta}$; the next section will be devoted to its consideration.

2.3 Elastic Energy Operator

The properties of the operator $\Phi^{\alpha\beta}(x, x')$ are in many aspects analogous to the properties of the operator $\Phi(x, x')$, which were considered in details in [Ref. 1.12, Sect. 2.4]. We shall therefore concentrate on features specific to the three-dimensional case.

Hermiticity. From (2.2.4), it follows that

$$\Phi^{\alpha\beta}(x, x') = \Phi^{\beta\alpha}(x', x), \quad \Phi^{\alpha\beta}(k, k') = \overline{\Phi^{\beta\alpha}(k', k)}. \tag{2.3.1}$$