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Differential pseudocontinua(*)

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IN THE PAPER a possibility of constructing differential pseudocontinuum models applicable to lattice dynamics is investigated. The relations between lattice force constants and coefficients of polynomial differential operator are found. Two theorems dealing with the asymptotic behaviour of lattice force constants are formulated and proved. Two examples are discussed in the harmonic approximation: a one-dimensional chain of atoms and a three-dimensional simple orthorhombic lattice. The obtained results are compared with those of the lattice dynamics theory.

W pracy zbadano możliwość konstrukcji różniczkowych modeli pseudocontinuum i ich zastosowań do opisu dynamiki sieci. Znaleziono związki pomiędzy stałymi siłowymi teorii sieci, a współczynnikami wielomianowego operatora różniczkowego. Sformułowano i udowodniono twierdzenia dotyczące asymptotycznego zachowania się stałych siłowych. Przedyskutowano dwa przykłady w przybliżeniu harmonicznym: jednowymiarowy łańcuch atomów i trójwymiarową prostą sieć rombową. Otrzymane wyniki porównano z teorią sieci.

В работе исследуется возможность построения дифференциальных псевдоконтинуальных моделей, применительно к описанию динамики решетки. Найдены соотношения между силовыми константами решетки и коэффициенты полиномиального дифференциального оператора. Сформулированы и доказаны утверждения об ассимптотическом поведении силовых констант. Обсуждаются два примера в гармоническом приближении: одномерная цепочка атомов и трехмерная простая ромбическая решетка. Результаты сравниваются с результатами полученными на основе теории решетки.

1. Introduction

APART from undoubtful successes, the lattice dynamics theory often encounters difficulties which are, in general, of a technical nature. First of all, there are troubles in applying discrete mathematics to a description of the behaviour of crystals. On the other hand the classical continuum approach does not allow to describe the phenomena which require consideration of small areas with diameters comparable with the interatomic distances.

Some expectations have been recently devoted to the theory called pseudo- or quasi-continuum which was developed by ROGULA [1] and KUNIN [2]. The main feature of the pseudocontinuum theory is the restriction of the set of admissible functions. These restricted *PC*-functions of the continuous argument uniquely interpolate the functions of the discrete argument. The mathematics of the pseudocontinuum theory is very flexible. In the framework of this theory, apart from discrete operators, differential or integral operators can also be used without losing their precise meaning.

In this paper we study the application of differential polynomial operators to describe the lattice dynamics. It is found that the force constant of a crystal lattice do not vanish

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identically for great distances but they tend to zero with some negative power of distance. In the Fourier K-space it corresponds to approximating the dispersion curves by polynomials.

The appropriate theorems about the admissible functions are formulated and proved and two examples are given. The obtained results are compared with those of the lattice dynamics theory.

2. Pseudocontinuum theory and differential operators

In this section we shall state briefly fundamental concepts of the pseudocontinuum theory as given by ROGULA [1] and KUNIN [2]. For the sake of consistency some slight changes in notation will be introduced. The wave vectors k are restricted to the reciprocal cell

The position of an atom in a three-dimensional primitive crystal lattice can be described by the vector

$$\mathbf{X}(\mathbf{n}) = A\mathbf{n}, \tag{2.1}$$

where $\mathbf{n}$ is a vector composed of the integers n_1, n_2, n_3, and A is a matrix whose elements are built up of the lattice constants a_1, a_2 and a_3.

In the continuum theory quantities such as displacements $\mathbf{u}(\mathbf{x})$ and forces $\mathbf{q}(\mathbf{x})$ are functions of a continuous variable $\mathbf{x}$ but in a crystal they have a physical meaning only in a discrete set of points

$$\mathbf{x} = \mathbf{X}(\mathbf{n}). \tag{2.2}$$

The set of these functions is too large and there are evident troubles in interpretating the results obtained. The goal of the pseudocontinuum theory was to find an appropriate class of functions. The admissible functions in the pseudocontinuum theory, the so-called PC- or QC-functions, are the entire analytic functions satisfying the inequality

$$|f(x)| \leqslant C(1+|x|)^N \exp\left(\frac{\pi}{a} Im x\right) \tag{2.3}$$

for certain constant C and N [5]. That is, they are of the order 1 and type π/a.

If f, $q \in PC$, then their convolution and all the derivatives are of the class PC. Also all polynomials are PC-functions.

The pseudocontinuum theory established a correspondence between the functions in discrete N-, continuous X- and Fourier K-representations. This can be done making use of the sampling function, the so-called Brillouin δ-function, which has the property

$$\delta_B(A\mathbf{n}) = \begin{cases} 1 & \text{for} \quad \mathbf{n} = 0, \\ 0 & \text{for} \quad \mathbf{n} \neq 0. \end{cases} \tag{2.4}$$

It has the following form resulting from the Fourier transformation method:

$$\delta_B(\mathbf{x}) = \frac{1}{(2\pi)^3} \int_B d^3k e^{i\mathbf{k}\mathbf{x}}, \tag{2.5}$$

where the integration extends over a certain volume B, e.g. the first Brillouin zone. In our case it will be the elementary cell of the reciprocal lattice. It is easy to see that the dimension of $\delta_B(\mathbf{x})$ is $[\mathrm{cm}^{-3}]$. The fundamental relations between the functions of one or two arguments and between the equations of motion on N-, X- and K-representations are given in [8].

In spite of the fact that the pseudocontinuum theory describes exactly the lattice dynamics, it admits differential equations of motion

$$\varrho\ddot{u}_i(\mathbf{x}, t)+P_{ij}(\partial)u_j(\mathbf{x}, t) = q_i(\mathbf{x}, t), \tag{2.6}$$

where $P_{ij}(\partial)$ is a differential polynomial in the partial derivative operators $\partial = (\partial_1, \partial_2, \partial_3)$

$$P_{ij}(\partial) = \sum_{0<|\mu|\leqslant s} a_{ij\mu}\partial^{\mu}. \tag{2.7}$$

Here $\mu = (\mu_1, \mu_2, \mu_3)$ is a multi-index described in [5]. Roughly speaking, it allows us to state how many indices take the values of 1, 2 and 3, respectively, instead of specifying the value of every index in an arbitrary tensor quantity of an arbitrary order symmetric in a certain group of indices. Thus we can write

$$\partial^{\mu} = \partial_1^{\mu_1}\partial_2^{\mu_2}\partial_3^{\mu_3}. \tag{2.8}$$

The value

$$|\mu| = \mu_1+\mu_2+\mu_3 \tag{2.9}$$

equals the number of tensor indices which correspond to the multi-index μ. The coefficient $a_{ij\mu}$ is equivalent to a tensor of the order $2+|\mu|$ symmetric in the last $|\mu|$ indices.

It was shown in [4] that every differential operator in the pseudocontinuum theory has an equivalent integral form. In fact, if we integrate by parts the following equality,

$$\partial_{\mathbf{x}}^{\mu}u_j(\mathbf{x}, t) = \int d^3x'\delta_B(\mathbf{x}-\mathbf{x}')\partial_{\mathbf{x}'}^{\mu}u_j(\mathbf{x}', t), \tag{2.10}$$

then we obtain

$$\varrho\ddot{u}_i(\mathbf{x}, t)+(-1)^{|\mu|}a_{ij\mu}\int d^3x'u_j(\mathbf{x}'t)\partial_{\mathbf{x}'}^{\mu}\delta_B(\mathbf{x}-\mathbf{x}') = q_i(\mathbf{x}, t), \tag{2.11}$$

and we can state that

$$\Phi_{ij}(\mathbf{x}, \mathbf{x}') = (-1)^{|\mu|}\Omega a_{ij\mu}\partial_{\mathbf{x}'}^{\mu}\delta_B(\mathbf{x}-\mathbf{x}'). \tag{2.12}$$

Equation (2.12) can be re-written in the K- and N-representations:

$$\Phi_{ij}(\mathbf{k}, \mathbf{k}') = (2\pi)^3\Omega a_{ij\mu}(i\mathbf{k}')^{\mu}\delta(\mathbf{k}-\mathbf{k}'), \tag{2.13}$$

$$\Phi_{ij}(\mathbf{n}, \mathbf{n}') = (-1)^{|\mu|}\Omega a_{ij\mu}\delta_B^{\mu}[A(\mathbf{n}-\mathbf{n}')], \tag{2.14}$$

where

$$\delta_B^{\mu}(\mathbf{x}) = \partial^{\mu}\delta_B(\mathbf{x}). \tag{2.15}$$

Equation (2.14) gives us the simple relation between the lattice force constants $\Phi_{ij}(\mathbf{n}, \mathbf{n}')$ and the coefficients of the differential polynomial operator $a_{ij\mu}$.

3. The asymptotics of the force constants

In contrast to usual approximations in the lattice theory, the force constants given by the formula (2.14) need not vanish identically for large distances. Instead of that they can, slower or faster, decrease. The asymptotical behaviour of the force constants is therefore crucial for the general applicability of differential pseudocontinuum models.

Before discussing this problem, it is necessary to establish some mathematical facts concerning the continuous-discrete Fourier transformation. For the sake of greater precision, in this paragraph we shall make use of different symbols for the function and its Fourier-image, e.g. f and $\hat{f}$, respectively. We shall start the discussion from the one-dimensional case.

3.1. One-dimensional row of atoms

Let B denote the open segment

$$k \in \left(-\frac{\pi}{a}, \frac{\pi}{a}\right), \tag{3.1}$$

and R — the entire real k-axis. Consider an admissible function $f(x)$, and let

$$f_n = f(an), \tag{3.2}$$

$$\hat{f}(\mathbf{k}) = a \sum_n e^{-iank} f_n. \tag{3.3}$$

The Fourier transform $\hat{f}$, considered on R, is a periodic function

$$\hat{f}\left(k+\frac{\pi}{a}\right) = \hat{f}\left(k-\frac{\pi}{a}\right) \tag{3.4}$$

or, more precisely, a periodic distribution (generalized function). If, for a certain l, the transform $\hat{f}$ is a function of the class $C^l(R)$, then

$$\begin{aligned} &\hat{f}\left(k+\frac{\pi}{a}-0\right) = \hat{f}\left(k-\frac{\pi}{a}+0\right), \\ &\hat{f}'\left(k+\frac{\pi}{a}-0\right) = \hat{f}'\left(k-\frac{\pi}{a}+0\right), \\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ &\hat{f}^{(l)}\left(k+\frac{\pi}{a}-0\right) = \hat{f}^{(l)}\left(k-\frac{\pi}{a}+0\right), \end{aligned} \tag{3.5}$$

for arbitrary k.

Let $\hat{f}(k)$ be an infinitely differentiable function of k on B. Then

$$anf_n = \frac{i}{2\pi} \int_{-\pi/a}^{\pi/a} dk e^{ikan} \hat{f}'(k) - \frac{i}{2\pi}(-1)^n \left[\hat{f}\left(\frac{\pi}{a}-0\right) - \hat{f}\left(-\frac{\pi}{a}+0\right)\right]. \tag{3.6}$$

By the Riemann-Lebesgue lemma for the integral in Eq. (3.6), one obtains the asymptotic expression for f_n:

$$f_n \approx \frac{c_n}{an} \quad \text{for} \quad n \to \infty, \tag{3.7}$$

where

$$c_n = \frac{i}{2\pi}\left(-1\right)^n\left[\hat{f}\left(\frac{\pi}{a}-0\right)-\hat{f}\left(-\frac{\pi}{a}+0\right)\right]+o(1), \tag{3.8}$$

is a bounded function of n.

If f is continuous, then the square bracket in the above equation vanishes. Instead of Eq. (3.6) we have

$$(an)^2 f_n = \frac{i^2}{2\pi}\int_{-\pi/a}^{\pi/a} dk e^{ikan}\hat{f}''(k) - \frac{i^2}{2\pi}(-1)^n\left[\hat{f}'\left(\frac{\pi}{a}-0\right)-\hat{f}'\left(-\frac{\pi}{a}+0\right)\right], \tag{3.9}$$

which implies

$$f_n \approx \frac{c_n}{(an)^2} \quad \text{for} \quad n\to\infty, \tag{3.10}$$

where

$$c_n = -\frac{1}{2\pi}(-1)^{n+1}\left[\hat{f}'\left(\frac{\pi}{a}-0\right)-\hat{f}'\left(-\frac{\pi}{a}+0\right)\right]+o(1). \tag{3.11}$$

By iterating the above procedure the following proposition is proven:

PROPOSITION 3.1. Let $\hat{f}(k)$ be $C^\infty(B)$ and $C^l(R)$ for a certain l. Then

$$f_n \approx \frac{c_n}{(an)^{2+l}} \quad \text{for} \quad n\to\infty, \tag{3.12}$$

where c_n is a bounded function of n.

3.2. Three-dimensional lattice

Let B denote the open Brillouin zone (or a reciprocal cell), and R^3- the entire real k-space. Then, for any admissible function $f(x)$ we have

$$f_{\mathbf{n}} = f(A\mathbf{n}), \tag{3.13}$$

$$\hat{f}(\mathbf{k}) = \Omega\sum_{\mathbf{n}}{}' e^{-i\mathbf{k}A\mathbf{n}} f_{\mathbf{n}}. \tag{3.14}$$

The periodicity condition of the Fourier transform $\hat{f}$ reads

$$\hat{f}(\mathbf{k}+\mathbf{K}/2) = \hat{f}(\mathbf{k}-\mathbf{K}/2), \tag{3.15}$$

for any reciprocal vector $\mathbf{K}$.

Let $\hat{f}_+(\mathbf{k})$ and $\hat{f}_-(\mathbf{k})$ be defined for $\mathbf{k}$ belonging to the boundary ∂B of the region B as outward and inward limit, respectively. If for a certain l the transform $\hat{f}(\mathbf{k})$ is of the class $C^l(R^3)$, then

$$\left[\left(\frac{\partial}{\partial k}\right)^\mu \hat{f}(\mathbf{k})\right]_+ = \left[\left(\frac{\partial}{\partial k}\right)^\mu \hat{f}(\mathbf{k})\right]_- \tag{3.16}$$

for arbitrary $k\in\partial B$ and arbitrary multi-index $|\mu|\leqslant l$. Equivalently

$$\left[\left(\frac{\partial}{\partial k}\right)^\mu \hat{f}(\mathbf{k}+\mathbf{K}/2)\right]_+ = \left[\left(\frac{\partial}{\partial k}\right)^\mu \hat{f}(\mathbf{k}-\mathbf{K}/2)\right]_+, \tag{3.17}$$

for

$$\mathbf{k}+\mathbf{K}/2 \in \partial B, \quad \mathbf{k}-\mathbf{K}/2 \in \partial B. \tag{3.18}$$

Instead of Eq. (3.6) we can now write

$$(\boldsymbol{\nu}A\mathbf{n})f_n = \frac{i}{(2\pi)^3}\int_B d^3k e^{i\mathbf{k}A\mathbf{n}}\left(\boldsymbol{\nu}\frac{\partial}{\partial \mathbf{k}}\right)\hat{f}(\mathbf{k}) - \frac{i}{(2\pi)^3}\int_{\partial B}(\boldsymbol{\nu}dS)e^{i\mathbf{k}A\mathbf{n}}\hat{f}_+(\mathbf{k}), \tag{3.19}$$

where $\boldsymbol{\nu}$ represents an arbitrary unit vector. Taking into account the central symmetry of B and following the argument of the previous subsection, we obtain the following:

PROPOSITION 3.2. Let $\hat{f}(\mathbf{k})$ be $C^\infty(B)$ and $C^l(R^3)$ for a certain l. Let $\boldsymbol{\nu}$ be an arbitrary unit vector. Then

$$f_n \simeq \frac{c_n(\boldsymbol{\nu})}{(\boldsymbol{\nu}A\mathbf{n})^{2+l}} \quad \text{for} \quad \mathbf{n}\to\infty \tag{3.20}$$

with $c_n(\boldsymbol{\nu})$ being a bounded function of $\mathbf{n}$.

4. One-dimensional chain

Let us consider an one-dimensional chain of atoms along the Ox axis (Fig. 1). The distance between the atoms is constant and equal to a. The equation of motion of such a model of crystal in the X-representation has the form

$$\varrho\ddot{u}(x,t)+\sum_\mu a_\mu \partial^\mu u(x,t) = q(x,t). \tag{4.1}$$

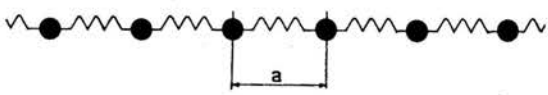

FIG. 1.

We assume that the crystal is homogeneous, thus $\varrho(x) = \varrho$ and

$$\partial a_\mu = 0, \tag{4.2}$$

which means that a_μ's are independent of the coordinate. The model is of course also centrosymmetric, and thus

$$a_\mu = 0 \quad \text{for odd } \mu. \tag{4.3}$$

The consequence of the above properties of the coefficients a is that the equation resulting from Eq. (2.12),

$$\Phi(\mathbf{x},\mathbf{x}') = a a_\mu \partial^\mu \delta_B(x-x'), \tag{4.4}$$

contains only derivatives of an even order. We restrict our considerations to the differential polynomial operator of the fourth order. Thus, on the basis of the one-dimensional form of the δ_B-function,

$$\delta_B(x) = \frac{1}{2\pi}\int_B dk e^{ikx} = \frac{1}{\pi x}\sin\frac{\pi x}{a}, \tag{4.5}$$

where B is an interval $[-\pi/a, \pi/a]$, we have to calculate the following four derivatives only:

$$
\begin{aligned}
\partial\delta_B(x) &= \frac{\cos\pi x/a}{ax} - \frac{\delta_B(x)}{x}, \\
\partial^2\delta_B(x) &= -\frac{\pi^2}{a^2}\,\delta_B(x) - 2\frac{\partial\delta_B(x)}{x}, \\
\partial^3\delta_B(x) &= -\frac{\pi^2}{a^2}\,\partial\delta_B(x) + \frac{2\pi^2}{a^2}\frac{\delta_B(x)}{x} + 6\frac{\partial\delta_B(x)}{x^2}, \\
\partial^4\delta_B(x) &= \frac{\pi^4}{a^4}\,\delta_B(x) + \frac{4\pi^2}{a^2}\frac{\partial\delta_B(x)}{x} - \frac{8\pi^2}{a^2}\frac{\delta_B(x)}{x^2} - 24\frac{\partial\delta_B(q)}{x^3}.
\end{aligned}
\tag{4.6}
$$

For $|x-x'| \neq 0$ we obtain

$$
\begin{aligned}
\Phi(x, x') &= a\left(a_2\,\partial^2\delta_B(x-x') + a_4\partial^4\delta_B(x-x')\right) \\
&= a\left(\frac{\cos\pi(x-x')/a}{a(x-x')^2}\left(2\frac{\pi^2}{a^2}a_4 - a_2\right) - 24a_4\frac{\cos\pi(x-x')/a}{a(x-x')^4}\right).
\end{aligned}
\tag{4.7}
$$

The one-dimensional form of Eq. (4.4) in the Fourier K-representation is as follows:

$$\Phi(k, k') = 2\pi a a_\mu (ik')^\mu \delta(k-k'). \tag{4.8}$$

The coefficient in Eq. (4.8) will be denoted by $W(k)$. It is easy to see that $W(k) = W(-k)$ identically for all k. It means that $W(k) \subset C^0(R)$.

Generally, for large $|x-x'|$ we have $W(\bar{x}) \sim 1/x^2$. Now, the question arises if one can choose the coefficients a_μ so that the relation $W(k) \subset C^1(R)$ is obtained. The answer is affirmative if we require the continuity of the first derivative of $W(k)$

$$W'(\pi/a) = W'(-\pi/a). \tag{4.9}$$

This condition yields

$$a_2 = (2\pi^2/a^2)a_4. \tag{4.10}$$

Because of the central symmetry we conclude that $W(k) \subset C^2$. According to the Proposition 3.1. $\Phi(x, x') \sim 1/x^4$.

Finally, we obtain the asymptotic behaviour of the lattice force constant in discrete N-representation:

$$\Phi(n, n') \approx \frac{24a_4\cos\pi(n-n')}{a^4(n-n')^4} \quad \text{for} \quad n \neq n'. \tag{4.11}$$

It is worth mentioning that since the factor $\cos(\pi n)$ equals $(-1)^n$, this asymptotic behaviour is oscillatory. As a consequence, in many situations the contributions of terms with large n's will approximately compensate each other.

5. Orthorhombic three-dimensional lattice

In this section we extend the results of the previous section to the three-dimensional case. We consider an infinite simple orthorhombic crystal lattice whose elementary cell is shown in Fig. 2.

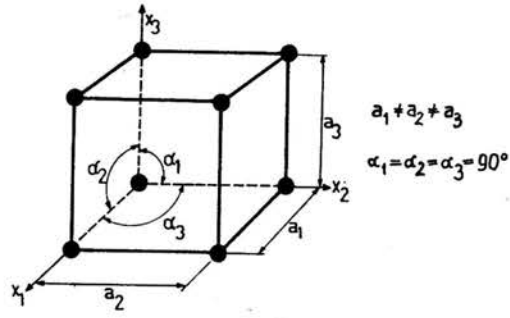

FIG. 2.

We assume that our crystal is homogeneous

$$\partial_k a_{ij\mu} = 0. \tag{5.1}$$

Since it is also centrosymmetric, then

$$a_{ij\mu} = 0 \quad \text{for odd} \quad |\mu|. \tag{5.2}$$

If we restrict the order of the differential polynomial operator to four, then, for $r = |\mathbf{x}-\mathbf{x}'| \neq 0$,

$$\Phi_{ij}(\mathbf{x}, \mathbf{x}') = \Omega a_{ij\mu} \partial^{\mu}_{\mathbf{x}'} \delta_B(\mathbf{x}-\mathbf{x}') = \Omega \Big[\sum_{|\mu|=2} a_{ij\mu} \partial^{\mu}_{\mathbf{x}'} \delta_B(\mathbf{x}-\mathbf{x}') + \sum_{|\mu|=4} a_{ij\mu} \partial^{\mu}_{\mathbf{x}'} \delta_B(\mathbf{x}-\mathbf{x}') \Big]. \tag{5.3}$$

For $|\mu| = 2$ we have the following μ's:

110 200
101 020
011 002

and for $|\mu| = 4$:

400	310	130	220	211
040	301	103	202	121
004	031	013	022	112

Totally it makes 21 terms.

Due to the translational symmetry of the reciprocal lattice, we have $\delta_B(\mathbf{x}) = \delta_B(x_1) \times \delta_B(x_2)\delta_B(x_3)$, where $\delta_B x_\gamma$ is given by the formula (4.5) and

$$\partial^{\mu} \delta_B(\mathbf{x}) = \partial_1^{\mu_1} \delta_B(x_1) \partial_2^{\mu_2} \delta_B(x_2) \partial_3^{\mu_3} \delta_B(x_3), \tag{5.4}$$

for the sake of convenience we shall write b_μ for $a_{ij\mu}$ and $W(\mathbf{k})$ for $\Phi_{ij}(\mathbf{k}, \mathbf{k}')$.

We require $W(\mathbf{k})$ to be at least of the class $C^0(R)$. This condition can be written as follows:

$$W(\mathbf{k})_{k_i = \pi/a_i} = W(\mathbf{k})_{k_i = -\pi/a_i}, \quad i = 1, 2, 3 \tag{5.5}$$

with respect to every component of the vector $\mathbf{k}$. The remaining two components of the vector $\mathbf{k}$ are arbitrary. The condition (5.5) implies vanishing of some group of b_μ. It is

easy to see that $W(\mathbf{x})$ behaves like $\sim 1/r^2$. According to Proposition 3.2, the smoothness of this function can be improved by increasing the order of $W(\mathbf{k})$. It appears that the coefficients b_μ can be chosen in such a manner that $W(\mathbf{k}) \subset C^1(R)$. This can take place when

$$W'_{k_i}(\mathbf{k})_{k_i=\pi/a_i} = W'_{k_i}(\mathbf{k})_{k_i=-\pi/a'_i} \quad i = 1, 2, 3. \tag{5.6}$$

The above conditions yield

$$\begin{aligned} &\frac{2\pi^2}{a_1^2} b_{400} - b_{200} = 0, \quad b_{310} = b_{130} = b_{301} = b_{103} = b_{013} = b_{031} = 0, \\ &\frac{2\pi^2}{a_2^2} b_{040} - b_{020} = 0, \quad b_{220} = b_{202} = b_{022} = 0, \\ &\frac{2\pi^2}{a_3^2} b_{004} - b_{002} = 0, \quad b_{112} = b_{121} = b_{211} = 0, \\ &\qquad\qquad b_{110} = b_{101} = b_{011} = 0. \end{aligned} \tag{5.7}$$

The obtained expression is symmetric and, according to Proposition 3.2, $\Phi_{ij}(\mathbf{k}, \mathbf{k}') \subset C^l$ where $l = 2$ and $\Phi_{ij}(\mathbf{x}, \mathbf{x}') \sim 1/r^4$.

Actually, the asymptotic behaviour of the lattice force constant in N-representation is as follows:

$$\begin{aligned} \Phi_{ij}(\mathbf{n}, \mathbf{n}') \cong -24\Omega \Bigg[&\frac{a_{ij400}}{a_1^5 (n_1 - n_1')^4} \cos\pi(n_1 - n_1') \delta_B(a_2(n_2 - n_2')) \delta_B(a_3(n_3 - n_3')) \\ &+ \frac{a_{ij040}}{a_2^5 (n_2 - n_2')^4} \cos\pi(n_2 - n_2') \delta_B(a_1(n_1 - n_1')) \delta_B(a_3(n_3 - n_3')) \\ &+ \frac{a_{ij004}}{a_3^5 (n_3 - n_3')^4} \cos\pi(n_3 - n_3') \delta_B(a_1(n_1 - n_1')) \delta_B(a_2(n_2 - n_2')) \Bigg]. \end{aligned} \tag{5.8}$$

6. Comparison with the lattice dynamics theory

In the previous section the asymptotic behaviour of the lattice force constants in the harmonic approximation for the considered models of crystals was found. The complete forms of the lattice force constant are as follows:

one-dimensional case:

$$\begin{aligned} \Phi(n, n') = aa_4 \Bigg[&-\frac{\pi^4}{a^4} \delta_B(a(n - n')) \\ &- \frac{24\delta_B^1(a(n - n')) + 8(\pi^2/a^2) a(n - n') \delta_B(a(n - n'))}{a^3 (n - n')^3} \Bigg], \end{aligned} \tag{6.1}$$

three-dimensional simple orthorhombic lattice:

$$\begin{aligned} \Phi_{ij}(n, n') = \Omega \Bigg[a_{ij400} \Bigg(&-\frac{\pi^4}{a_1^4} \delta_B(a_1(n_1 - n_1')) \\ &- \frac{24\delta_B^1(a_1(n_1 - n_1')) + 8(\pi^2/a_1^2) a_1(n_1 - n_1') \delta_B(a_1(n_1 - n_1'))}{a_1^3 (n_1 - n_1')^3} \Bigg) \\ &\times \delta_B(a_2(n_2 - n_2')) \delta_B(a_3(n_3 - n_3')) + \text{cyclic terms} \Bigg], \end{aligned} \tag{6.2}$$

where $\delta_B^1(a(n-n'))$ is understood in the sense of Eqs. (2.14) and (2.15) and, in Eq. (6.2), for cyclic terms one should put the corresponding expressions with indices permuted, like in Eq. (5.8).

In the lattice dynamics theory, if one expands the potential energy of the crystal Φ about the equilibrium positions of the atoms, then the first non-trivial term is

$$\Phi_2 = \frac{1}{2!} \sum_{\substack{\mathbf{m}i \\ \mathbf{n}j}} \Phi_{ij}^{\mathbf{mn}} u_j^{\mathbf{n}} u_j^{\mathbf{n}}, \tag{6.3}$$

where the primitive lattice force constants $\Phi_{ij}^{\mathbf{mn}}$ equal $\Phi_{ij}(\mathbf{n}, \mathbf{n}')$. It is well known [6] that the lattice force constants have to fulfil certain invariance relations. The following invariance relations resulting from the translational invariance of the crystal

$$\Phi_{ij}^{\mathbf{mn}} = \Phi_{ji}^{\mathbf{nm}}, \tag{6.4}$$

$$\sum_{\mathbf{m}} \Phi_{ij}^{\mathbf{mn}} = 0 \quad \text{for every } n, i, j, \tag{6.5}$$

$$\Phi_{ij}^{\mathbf{mn}} = \Phi_{i}^{\mathbf{m}+\mathbf{h}\,\mathbf{n}+\mathbf{h}} = \Phi_{i}^{\mathbf{0}\,\mathbf{n}-\mathbf{m}} = \Phi_{i}^{\mathbf{m}-\mathbf{n}\,\mathbf{0}}, \tag{6.6}$$

where $\mathbf{h}$ is the translational vector of the lattice, and

$$\Phi_{ij}^{\mathbf{mn}} = \Phi_{i}^{-\mathbf{m}-\mathbf{n}} = \Phi_{ij}^{\mathbf{nm}} = \Phi_{ji}^{\mathbf{mn}}, \tag{6.7}$$

are fulfilled automatically. Equation (6.6) means that $\Phi_{ij}(\mathbf{n}, \mathbf{n}') = \Phi_{ij}(\mathbf{n}-\mathbf{n}')$. As an example we shall show that Eq. (6.5) is valid in our model. For simplicity we shall carry out our considerations by making use of the one-dimensional $\Phi(\mathbf{n}, \mathbf{n}')$.

It is easy to show that

$$\lim_{x\to 0} \partial^2 \delta_B(x) = -\frac{1}{3}\frac{\pi^2}{a^2}, \quad \lim_{x\to 0} \partial^4 \delta_B(x) = \frac{1}{5}\frac{\pi^4}{a^4}. \tag{6.8}$$

Equations (6.8) yield

$$\lim_{n\to 0} \Phi(n) = -aa_4 \frac{7}{15}\frac{\pi^4}{a^4}. \tag{6.9}$$

If we make use [7] of the relation

$$\sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^{2n}} = \frac{(2^{2n-1}-1)\pi^{2n}}{(2n)!} |B_{2n}|, \tag{6.10}$$

where in our case $n = 2$ and B_4, the Bernoulli number, is equal to $-1/30$, then

$$2\sum_{n-1}^{\infty} \Phi(n) = aa_4 \frac{7}{15}\frac{\pi^4}{a^4}, \tag{6.11}$$

and finally

$$\sum_{n} \Phi(n) = \Phi(0) + 2\sum_{n=1}^{\infty} \Phi(n) = 0. \tag{6.12}$$

The invariance relations resulting from rotational symmetry of the three-dimensional crystal lattice

$$\sum_{\mathbf{m}} \Phi^{\mathbf{mn}}_{ik} X^{\mathbf{m}}_{j} = \sum_{\mathbf{m}} \Phi^{\mathbf{mn}}_{jk} X^{\mathbf{m}}_{i} \quad \text{for every } \mathbf{n}, i, j, k, \tag{6.13}$$

are also fulfilled.

On the basis of the above discussion we can state that the proposed differential pseudocontinuum models describe crystal dynamics at the same level of accuracy and consistency as the classical discrete theory. Nevertheless, there is an important difference between these two approaches. In applications of the classical lattice dynamics it is usually assumed that the force constants vanish identically for sufficiently great distances between atoms. This is not the case in our approach. The force constants derived from a differential pseudocontinuum do not vanish identically but tend asymptotically to zero with a certain nega-

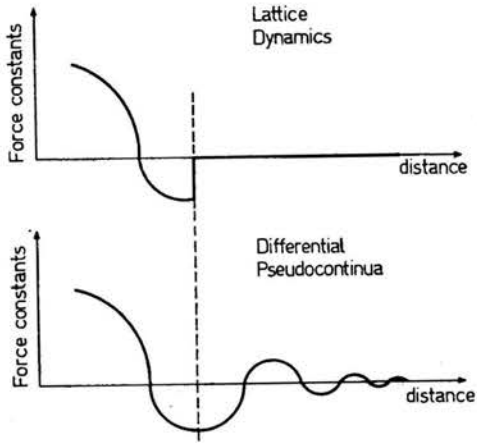

FIG. 3.

tive power of distance, as illustrated in Fig. 3. The asymptotic decrease of the force constants with the distance can be made faster by making use of the differential operators of higher order.

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