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Mechanical models for lattice vibrations

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THE TRANSVERSE lattice vibrations of a mechanical model which consists of a one-dimensional chain of pair of masses is studied. The masses with different moments of inertia are connected by massless beams and are also influenced by transverse forces. A transverse wave moves along the chain and causes transverse displacements and rotations of the masses. The discrete equations of motion and the dispersion relations are derived. By a limit procedure the discrete equations of motion are transformed to continuous ones. The results are then applied to KNO_3.

Zbadano drgania poprzeczne sieci w modelu mechanicznym stanowiącym jednowymiarowy łańcuch par mas skupionych. Masy o różnych momentach bezwładności połączone są nieważkimi prętami i poddane również działaniu sił poprzecznych. Fala poprzeczna posuwając się wzdłuż łańcucha wywołuje przemieszczenia poprzeczne i obroty poszczególnych mas. Wyprowadzono dyskretne równania ruchu i związki dyspersyjne. Przejście graniczne przekształca równania ruchu na zależności kontynualne. Wyniki zastosowano do KNO_3.

Исследованы поперечные колебания решетки в механической модели, составляющей одномерную цепь пар сосредоточенных масс. Массы с разными моментами инерции соединены невесомыми стержнями и подвергнуты тоже действию поперечных сил. Поперечная волна, двигаясь вдоль цепи, вызывает поперечные перемещения и вращения отдельных масс. Выведены дискретные уравнения движения и дисперсионные соотношения. Предельный переход превращает уравнения движения в континуальные зависимости. Результаты применены к KNO_3.

1. Introduction. The mechanical model

THE IDEA of investigating discrete and continuous mechanical models for some special lattice vibrations came to me upon reading A. ASKAR'S [1, 2] and I. FISCHER-HJALMAR'S

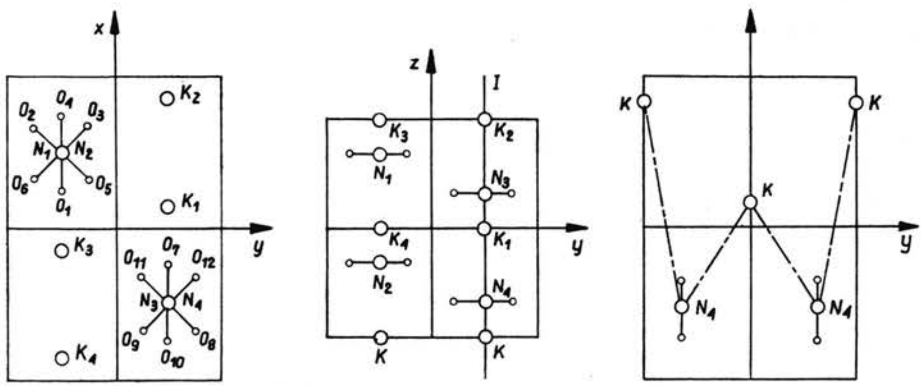

FIG. 1.

[3, 4] works on the KNO_3 crystal. The continuous model is compared with the micropolar theory.

The unit cell of KNO_3 in its aragonite structure is shown in Fig. 1. The left and the middle figures show four molecules in the unit cell and orthorhombic symmetry. Therefore waves travelling along the three orthogonal axes (x, y, z) are uncoupled.

In the mechanical models we consider the case of a transverse wave travelling along z, that is along the zigzag-shaped chain of ions about the I axis, transverse displacements along y, and rotations around x are assumed.

In ASKAR's discrete mechanical model, see [1], the ions K^+ and NO_3^- are considered as rigid bodies, the chain is made linear, the ions are joined by massless beams, which cause coupling between transverse displacements and rotations. Furthermore there are transverse forces on the ions from the chains in the neighbourhood. This means that a transverse acoustical, a transverse optical and a rotational mode are obtained.

In the mechanical discrete model discussed here we consider a more general case with two rigid bodies whose masses are M_1 respectively M_2 and moments of inertia J_1 respectively J_2, see Fig. 2. In this model the chain is simplified to be linear with constant dis-

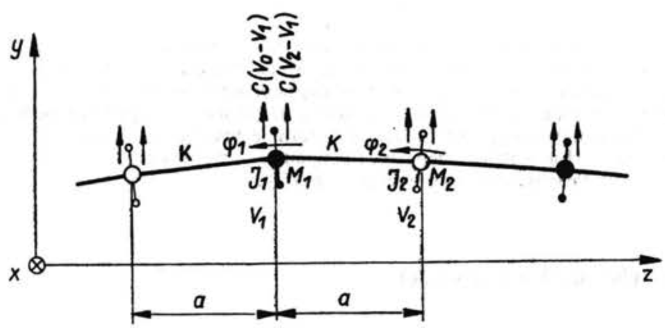

FIG. 2.

tances a between the masses. These are joined by identical massless beams with the bending spring constant K. Furthermore every mass is acted on by a pair of transverse forces assiociated with the spring constant C. Transverse displacements are indicated by v_i and rotations by φ_i. Especially for KNO_3 we have that $M_1 \Leftrightarrow NO_3^-$, $M_2 \Leftrightarrow K^+$ and J_2 vanishes.

The aim of this investigation is to derive from the equations of motion of the discrete model the corresponding equations of motion of a continuous model. The last equations are when J_2 vanishes compared with equations of motion obtained from the micropolar theory, see [3].

Of course this simplified model can give only qualitative results, for example for crystals. In the case J_2 vanishes, a similar but better model is presented by I. FISCHER-HJALMARS in [4].Wave solutions for discrete models similar to the ones above and corresponding continuum models are given in [5].

2. Derivation of the continuous model

At first the equations of the discrete model are shown, see [1], which are linear difference equations:

$$M_1\ddot{v}_1 = (C+K)(v_2+v_0-2v_1)+\frac{1}{2}Ka(\varphi_2-\varphi_0), \tag{2.1}$$

$$M_2\ddot{v}_2 = (C+K)(v_3+v_1-2v_2)+\frac{1}{2}Ka(\varphi_3-\varphi_1), \tag{2.2}$$

$$J_1\ddot{\varphi}_1 = \frac{1}{2}Ka(v_0-v_2)-\frac{1}{6}Ka^2(\varphi_2+\varphi_0-4\varphi_1), \tag{2.3}$$

$$J_2\ddot{\varphi}_2 = \frac{1}{2}Ka(v_1-v_3)-\frac{1}{6}Ka^2(\varphi_3+\varphi_1-4\varphi_2). \tag{2.4}$$

As the continuous model is valid only for long waves ($aq \ll 1, q =$ wave number), compare [5], we derive the equations of motion for long waves of the discrete model with Taylor series expansions and retaining derivatives up to the second order. We obtain now the following linear differential equations:

$$M_1\ddot{v}_1 = (C+K)(2v_2+a^2v_{2,33}-2v_1)+Ka^2\varphi_{2,3}, \tag{2.5}$$

$$M_2\ddot{v}_2 = (C+K)(2v_1+a^2v_{1,33}-2v_2)+Ka^2\varphi_{1,3}, \tag{2.6}$$

$$J_1\ddot{\varphi}_1 = -Ka^2v_{2,3}-\frac{2}{3}Ka^2\varphi_1-\frac{1}{3}Ka^2\varphi_2-\frac{1}{6}Ka^4\varphi_{2,33}, \tag{2.7}$$

$$J_2\ddot{\varphi}_2 = -Ka^2v_{1,3}-\frac{2}{3}Ka^2\varphi_2-\frac{1}{3}Ka^2\varphi_1-\frac{1}{6}Ka^4\varphi_{1,33}. \tag{2.8}$$

With wave solutions as $e^{i(qz-\omega t)}$ an acoustical mode, an optical mode and two rotational modes are obtained. Then we can calculate the following dispersion relations and amplitude relations:

Acoustical mode

$$\omega_{\mathrm{ac}}^2 = \frac{2C}{M_1+M_2}a^2q^2, \tag{2.9}$$

$$\frac{v_1}{v_2} = 1+O(a^2q^2), \quad \frac{\varphi_1}{v_1} = O(aq), \quad \frac{\varphi_2}{v_1} = O(aq). \tag{2.10}$$

Optical mode

$$\omega_{\mathrm{opt}}^2 = 2(C+K)\left(\frac{1}{M_1}+\frac{1}{M_2}\right)+O(a^2q^2), \tag{2.11}$$

$$\frac{v_1}{v_2} = -\frac{M_2}{M_1}+O(a^2q^2), \quad \frac{\varphi_1}{v_1} = O(aq), \quad \frac{\varphi_2}{v_1} = O(aq). \tag{2.12}$$

Rotational modes

$$\omega_{\mathrm{rot}\,1,2}^2 = \frac{1}{3}\frac{Ka^2}{J_1}\frac{J_1}{J_2}+1\mp\left(\left(\frac{J_1}{J_2}\right)^2-\frac{J_1}{J_2}+1\right)^{1/2}+O(a^2q^2), \tag{2.13}$$

$$(2.14)\quad \frac{\varphi_1}{\varphi_2} = \frac{\dfrac{J_2}{J_1} \mp \left(\left(\dfrac{J_2}{J_1}\right)^2 - \dfrac{J_2}{J_1} + 1\right)^{1/2}}{\dfrac{J_1}{J_2} \mp \left(\left(\dfrac{J_1}{J_2}\right)^2 - \dfrac{J_1}{J_2} + 1\right)^{1/2}} + O(a^2q^2), \quad \frac{v_1}{\varphi_1} = O(aq), \quad \frac{v_2}{\varphi_1} = O(aq).$$

For vanishing J_2 we obtain only one rotational mode with $\omega_{\text{rot}1} = \dfrac{1}{2}\dfrac{Ka^2}{J_1}$ while $\omega_{\text{rot}2} \to \infty$.

We shall derive continuous equations of motion comparable with the differential equations of the discrete model. We transform the discrete model to a continuous one by some limit procedures. Those are chosen in such a way that the following conditions are fulfilled:

1. The density $\varrho' = \dfrac{M_1+M_2}{2a}$ must be finite.

2. The dispersion relations $\omega_{\text{ac}}(q)$ and $\omega_{\text{rot}1,2}(q)$ must be identical in both models.

We let a vanish, and the following terms must remain finite and unchanged compared with the discrete model:

$$(2.15)\qquad \frac{M_1}{a}, \ \frac{M_2}{a}, \ \frac{J_1}{a}, \ \frac{J_2}{a}, \ Ca, \ Ka.$$

We make the following variable transformations in the discrete equations of motion:

$$(2.16)\qquad u = v_1 - v_2, \quad v = \frac{M_1 v_1 + M_2 v_2}{M_1 + M_2}, \quad \psi_1 = \varphi_1 + \varkappa\varphi_2, \quad \psi_2 = \gamma\varphi_1 + \varphi_2.$$

The limit procedures are inserted, what means that a lot of terms vanish, and we obtain the following continuous equations of motion:

$$(2.17)\qquad \frac{M_1+M_2}{2a}\ddot{v} + (Ca+Ka)v_{,33} + \frac{1}{2}Ka\left[\frac{\gamma-1}{\gamma\varkappa-1}\psi_{1,3} + \frac{\varkappa-1}{\gamma\varkappa-1}\psi_{2,3}\right],$$

$$(2.18)\qquad \frac{J_1J_2}{a^2}\ddot{\psi}_1 = -Ka\left(\varkappa\frac{J_1}{a} + \frac{J_2}{a}\right)v_{,3} - \frac{1}{3}Ka\left[\frac{J_1(2\gamma\varkappa-\varkappa)+J_2(\gamma-2)}{a(\gamma\varkappa-1)}\psi_1 + \frac{J_1(\varkappa^2-2\varkappa)+J_2(2\varkappa-1)}{a(\gamma\varkappa-1)}\psi_2\right],$$

$$(2.19)\qquad \frac{J_1J_2}{a^2}\ddot{\psi}_2 = -Ka\left(\frac{J_1}{a} + \gamma\frac{J_2}{a}\right)v_{,3} - \frac{1}{3}Ka\left[\frac{J_1(2\gamma-1)+J_2(\gamma^2-2\gamma)}{a(\gamma\varkappa-1)}\psi_1 + \frac{J_1(\varkappa-2)+J_2(2\gamma\varkappa-1)}{a(\gamma\varkappa-1)}\psi_2\right].$$

For the continuous model finally the following results are obtained:

1. The optical mode will disappear as $\omega_{\text{opt}} \to \infty$.

2. The dispersion relations $\omega_{\text{ac}}(q)$ and $\omega_{\text{rot}1,2}\ (q)$ are identical for both models if J_1 respectively J_2 are modified, considering the q^2-term in $\omega_{\text{rot}1,2}$.

3. The amplitude relations are identical for both models when q vanishes, but they differ more and more for increasing q.

Furthermore we observe that this continuous model is not a real continuum model which would give the acoustical mode only, compare [5].

3. Comparison with the micropolar theory

From the micropolar theory we obtain the following equations of motion:

$$\varrho'\ddot{v}' = \left(c' + \frac{1}{4}k'\right)v'_{,33} + \frac{1}{2}k'\varphi'_{,3}, \tag{3.1}$$

$$\varrho' j'\ddot{\varphi}' = -k'\varphi' + \alpha'\varphi'_{,33} - \frac{1}{2}k'v'_{,3}, \tag{3.2}$$

ϱ' — mass density, j' — moment of inertia/mass unit, c' — symmetric stress coefficient, k' — antisymmetric stress coefficient, α' — couple stress coefficient, v' — transverse displacement, φ' — microrotation.

These equations give one acoustical mode and one rotational mode. This corresponds to the case in the continuous model discussed above where J_2 vanishes.

This case is obtained if we insert $\gamma = \varkappa = 0$ and let J_2 vanish in the corresponding equations of motion.

$$\frac{M_1 + M_2}{2a}\ddot{v} = \left[Ca + \frac{1}{4}Ka\right]v_{,33} + \frac{1}{4}Ka\varphi_{,3}, \tag{3.3}$$

$$\frac{J_1}{a}\ddot{\varphi} = -\frac{1}{2}Kav_{,3} - \frac{1}{2}Ka\varphi. \tag{3.4}$$

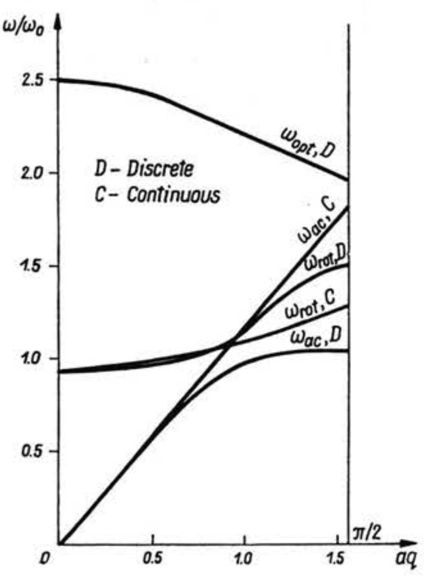

FIG. 3.

v — transverse displacement of the mass center of two neighbouring masses, φ — rotation of the mass with J_1.

Now we identify these equations with the previous micropolar equations and obtain

$$(3.5)\qquad \varrho' = \frac{M_1+M_2}{2a}, \quad \varrho' j' = 2\frac{J_1}{a}, \quad c' = Ca, \quad k' = Ka,$$

$$\alpha' = 0 \text{ (no couple stress)}, \quad v' = v, \quad \varphi' = \frac{1}{2}\varphi.$$

The dispersion relations for KNO_3 are calculated both from the discrete difference equations and from the derived continuous equations. In [1] we have M_1, M_2, J_1 and a determined from the crystallography, C and K from experimental values on ω_{rot} and ω_{opt} for long waves. This is shown in Fig. 3.

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