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The generalized pendulum analogy of the X-ray dynamical diffraction by one-dimensional regularly deformed crystals

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The pendulum analogy has been generalized in a form suitable for the case of an off-Bragg position. It is shown that, by introducing a time variation of the pendula masses, this analogy can be supplied to simulate the X-ray dynamical diffraction by a one-dimensional regularly deformed crystal. The correspondence between the adiabatic invariants of the new mechanical system and the invariants of the Eikonal approximation of the X-ray dynamical theory is established

1. Introduction

The mechanical system of two coupled pendula is a very helpful analogy in X-ray dynamical diffraction. The well known interpretation of the *Pendellösung* phenomenon as a beating process follows from this analogy. However, the original mechanical system proposed by Ewald (1965) is not suitable in the case of an off-Bragg position and cannot take into account a regular crystal deformation. (By a regular deformation, we mean a bending, a single dislocation, an acoustic wave *etc.*) Therefore, the generalization of the mechanical system and of the pendulum analogy is a problem of interest in X-ray dynamical diffraction by regularly deformed crystals. It is possible that new physical approaches to various important aspects of the dynamical theory, such as interbranch scattering, might be obtained with the help of a generalized pendulum analogy. In this paper, we consider a mechanical system corresponding to the case of one-dimensional (1D) regular deformations. The adiabatic invariance of this mechanical system is examined and it allows us to analyse in detail the invariants of the Eikonal approximation of the X-ray dynamical theory, in the case of a slightly deformed crystal (Kato, 1963*a*).

2. Generalized pendulum analogy and local corresponding relations

Let us consider the mechanical system of two coupled pendula. However, in contradiction to the Ewald model, we assume that the pendula masses $m_{1,2}$ can be different from each other and that they depend on the time t. Without any loss of generality, we choose $m_2 > m_1$. Then, the appropriate Lagrange function can be represented in the following form:

$$L = \dot{\varphi}_1^2/\omega_1^2 + \dot{\varphi}_2^2/\omega_2^2 - \omega_0^2(\varphi_1^2/\omega_1^2 + \varphi_2^2/\omega_2^2) - (\varphi_1 - \varphi_2)^2. \quad (1)$$

Here $\varphi_{1,2}$ are the pendula angle variables, $\omega_0 = (g/l)^{1/2}$ and $\omega_{1,2} = (\kappa/m_{1,2})^{1/2}$, where g, κ and l stand for the acceleration of gravity, the coefficient of elasticity of the coupling and the length of the pendula, respectively. Using the present mechanical model, we can generalize the pendulum analogy of the X-ray dynamical diffraction in the case of an off-Bragg position. For this purpose, we will establish a correspondence between the parameters of the mechanical system and the parameters of the X-ray dynamical diffraction theory. We will transform the equations of motion following from (1) to the Takagi–Taupin form, considering a sufficiently small time interval, Δt, within which the masses $m_{1,2}$ can be regarded as constants. Furthermore, in view of a weak coupling between the pendula, it is possible to neglect the second-order derivatives in these equations of motion. It is necessary to carry out the change of the variables $\varphi_{1,2}$ for 'slow' variables $\tilde{\varphi}_{1,2}$ by means of the following relations for it:

$$\varphi_{1,2} = (m_{1,2})^{-1/2} \exp\{-i\omega_H t\}\tilde{\varphi}_{1,2}. \quad (2)$$

In expressions (2), we extracted the 'sharp' vibrations with high frequency $\omega_H = \omega_0 + (4\omega_0)^{-1}(\omega_1^2 + \omega_2^2)$ from the amplitudes $\varphi_{1,2}$. Consequently, to determine the local corresponding relations, we have the following equations of motion:

$$\dot{\tilde{\varphi}}_{1,2} = \frac{i\omega_1\omega_2}{2\omega_0}\tilde{\varphi}_{2,1} \mp \frac{i(\omega_1^2 - \omega_2^2)}{4\omega_0}\tilde{\varphi}_{1,2}. \quad (3)$$

In the case of symmetric transmission and a 1D regularly deformed crystal, we can write the Takagi–Taupin equations in the form:

$$\frac{\mathrm{d}D_{0,h}}{\mathrm{d}z} = -\frac{i\pi}{\xi_h} D_{h,0} \exp\{\pm i\mathbf{hu}\} - \frac{i\pi}{\xi_0} D_{0,h}. \quad (4)$$

Here, $D_{0,h}$, $\mathbf{h}$, $\mathbf{u}$, ξ_0 and ξ_h stand for the amplitudes of the transmitted and diffracted waves, the diffraction vector, the displacement field oriented along the surface and the extinction lengths in the forward and diffraction directions, respectively. Moreover, we suppose that the displacement field $\mathbf{u}$ and, consequently, the amplitudes $D_{0,h}$ depend on the crystal depth, which is denoted by the z coordinate. Introduce into consideration the following momenta:

$$Q_0 = k\cos\theta_B \quad \text{and} \\ Q_{1,2} = \{k\cos\theta_B[\pm W + (W^2 + 4\pi^2/\xi_h^2)^{1/2}]\}^{1/2}, \tag{5}$$

where k, θ_B, W are the wave number of the incident wave, the Bragg angle, a Bragg deviation parameter (positive, for definiteness), respectively. With the help of these expressions and of the substitutions

$$D_{0,h} = \exp\{\pm i\pi/2 \pm ihu/2 - i\pi z/\xi_0\}\tilde{D}_{0,h},$$

equations (4) can be represented as follows:

$$\frac{d\tilde{D}_{0,h}}{dz} = \frac{iQ_1Q_2}{2Q_0}\tilde{D}_{h,0} \mp \frac{i(Q_1^2 - Q_2^2)}{4Q_0}\tilde{D}_{0,h}. \tag{6}$$

Comparing (6) and (3), we can find the desirable corresponding relations, which have the form

$$\tilde{\varphi}_{1,2} \to \tilde{D}_{0,h} \quad \text{and} \quad \omega_0 \to Q_0, \quad \omega_{1,2} \to Q_{1,2}. \tag{7}$$

As follows from (7) and (5), the deviation from the Bragg law, which is determined by W, is equivalent to the difference between m_1 and m_2. This means that we can accept $W > 0$, if $m_2 > m_1$ and $W < 0$ in the opposite case. Then, the larger frequency among $\omega_{1,2}$ will correspond to the larger momentum among $Q_{1,2}$. Obviously, in accordance with the developed analogy, the variation of the ratio m_2/m_1 leads to moving the tiepoints along the branches of the dispersion surface. In the limiting case $m_2/m_1 \gg 1$, which corresponds to strong deformations, we have $Q_1/Q_2 \gg 1$ or $W \gg \xi_h^{-1}$. It should be pointed out that the dynamical coupling between pendula is then broken and the refraction regime happens under such conditions. Clearly, by supposing the masses $m_{1,2}$ constant for any time, we can describe the case of an off-Bragg position for an ideal crystal. At the same time, as seen from (7), we are able to simulate the X-ray dynamical diffraction by a 1D regularly deformed crystal by introducing a time variation of the pendula masses.

3. The adiabatic invariance and the Eikonal approximation for X-ray dynamical diffraction

As is well known, the conception of adiabatic invariance may be applied to any mechanical system under sufficiently slow variations of its parameters. In this connection, it is sensible to study this point for the generalized pendulum model and to find the appropriate analogy for the X-ray dynamical diffraction by a regularly deformed crystal. To determine the adiabatic invariants of the proposed mechanical system, it is very suitable to use the Lagrange formalism. For this purpose, we diagonalize the Lagrange function (1) and modify the equations of motion, which are obtained in so doing, to harmonic form. It is not difficult to establish that such modifications can be easily realized by means of the following changes of the variable t in the equations of motion:

$$\begin{cases} d\tau_1 = \dfrac{\omega_0}{2\omega_B}\,dt & (8) \\ d\tau_2 = \dfrac{\omega_2^2}{\omega_1^2}\dfrac{\omega_0}{2\omega_B}\,dt. & (9) \end{cases}$$

Here, $\omega_B = (\omega_1^2 + \omega_2^2)/(2\omega_0)$ is the beat frequency, where $\omega_B << \omega_0$, and $\tau_{1,2}$ are the new time variables corresponding to the following equations of motion:

$$\frac{d^2\psi_{1,2}}{d\tau_{1,2}^2} + \Omega_{1,2}^2(\tau_{1,2})\psi_{1,2} = 0, \tag{10}$$

where $\Omega_1(\tau_1) = 2\omega_B(\tau_1)$ and

$$\Omega_2(\tau_2) = 2\omega_B(\tau_2)\frac{\omega_1^2(\tau_2)}{\omega_2^2(\tau_2)}[1 + 2\omega_B(\tau_2)/\omega_0]^{1/2};$$

$\psi_{1,2}$ are the main coordinates for the Lagrange function, which are related to variables $\varphi_{1,2}$ as follows:

$$\begin{cases} \psi_1 = \dfrac{\omega_2^2}{2\omega_0\omega_B}\varphi_1 + \dfrac{\omega_1^2}{2\omega_0\omega_B}\varphi_2 & (11) \\ \psi_2 = \dfrac{\omega_2^2}{2\omega_0\omega_B}(\varphi_1 - \varphi_2). & (12) \end{cases}$$

As is well known (Landau & Lifshitz, 1988), equations (10) determine the motion under which the action variables are conserved in the case of adiabatic slow variations of the frequencies $\Omega_{1,2}$ (or masses $m_{1,2}$). Consequently, the adiabatic invariants $I_{1,2}$ are of the form

$$I_{1,2} = \langle E\rangle_{1,2}/\Omega_{1,2}. \tag{13}$$

Here, $\langle E\rangle_{1,2} = (1/T_{1,2})\int_0^{T_{1,2}} E(\tau_{1,2})\,d\tau_{1,2}$ are averaged energies and $T_{1,2} = 2\pi/\Omega_{1,2}$ are periods of motion in $\tau_{1,2}$. Using expressions (8), (9) and (2), (11), (12), we will calculate the invariants $I_{1,2}$ as functions of $\tilde{\varphi}_{1,2}$ and t. We will take into account that functions $\tilde{\varphi}_{1,2}$, as solutions of the equations of motion (3), are superpositions of two modes. In the vicinity of any time t, the ratios $\xi^{\pm}$ of the amplitudes of these modes $\tilde{\varphi}_2^{\pm}$ and $\tilde{\varphi}_1^{\pm}$ satisfy the relations

$$\xi^{\pm} = \pm\omega_{1,2}/\omega_{2,1}, \tag{14}$$

where signs + and − specify the upper and lower modes, respectively. After a straightforward calculation, with the help of expressions (14), we obtain the resultant expressions for $I_{1,2}$ (up to constant factor):

$$I_{1,2} = \omega_0(1 + \omega_{1,2}^2/\omega_{2,1}^2)|\tilde{\varphi}_1^{\pm}|^2. \tag{15}$$

Obviously, if we divide the time interval ΔT into sufficiently small subintervals Δt_i, then expressions (15) will be satisfied within Δt_i too. It follows from this that the appropriate invariants for the X-ray dynamical diffraction by a 1D regularly deformed crystal can be determined by means of the local correspondence relations (7). As is easily seen, these invariants denoted by $J_{1,2}$ have the form

$$J_{1,2} = k\cos\theta_B(1 + Q_{1,2}^2/Q_{2,1}^2)|D_0^{\pm}|^2, \tag{16}$$

where D_0^+ and D_0^- are the amplitudes of the transmitted wavefields for the 'upper' and 'lower' branches of the dispersion surface, respectively. As appears from (6), in the vicinity of any z the expressions for the ratios of the appropriate amplitudes of the transmitted and diffracted waves corresponding to the same branch of the dispersion surface are analogous to the ratios (14). Using this fact and expressions (16), we can calculate the new ratios between the amplitudes $D^{\pm}_{0,h}$:

$$P_{1,2} = \frac{Q_{1,2}|D^{+}_{0,h}|}{Q_{2,1}|D^{-}_{0,h}|} \quad \text{and} \quad R_{1,2} = \frac{|D^{+}_{0,h}|}{|D^{-}_{h,0}|},$$

where $P_{1,2}$ and $R_{1,2}$ are constants, which can be obviously considered as invariants too. However, it is necessary to remark that two adiabatic invariants only will be independent among the described constants. Clearly, these invariants are conserved only under sufficiently smooth deformations which correspond to adiabatic slow variations of the parameters of the mechanical system. This suggests that such invariants are conserved within the Eikonal approximation of the dynamical theory, which is valid in the case of sufficiently smooth deformations. Using the results obtained by Molodkin & Shevchenko (2002), with the help of the 'lamella' model of a deformed crystal (Authier, 1961; Kato, 1963*b*), it is possible to verify this suggestion. According to these results, the normal to crystal surface components $\mathbf{S}^{\pm}$ of the Poynting vector averaged over the period of *Pendellösung*, which correspond to different branches of the dispersion surface, are invariants in the Eikonal approximation and equal to constants $J_{1,2}$, respectively. Thus, applying the local corresponding relations (7), we can transform the adiabatic invariants of the generalized pendulum model to invariants of the Eikonal approximation of the X-ray dynamical theory. Besides, we can also show that the condition of the adiabatic invariance for the coupled pendula corresponds to the condition of validity of the Eikonal approximation. Indeed, the condition of applicability of the adiabatic invariance conception for pendula has the following form:

$$\mathrm{d}\lambda/\mathrm{d}\tau_{1,2} \ll \lambda/T_{1,2}, \tag{17}$$

where we can accept $\lambda = (\omega_1^2 + \omega_2^2)/(2\omega_0)$. Multiplying the small factor ω_B/ω_0 with the right-hand side of the inequality (17), we obtain the inequality describing the sufficiently slow disturbances of the pendulum vibrations in the regime of the adiabatic invariance. Using the expressions (8), (9) within a small interval Δt, where we can set $t \to z$ and apply the local corresponding relations (7), it is possible to obtain the following inequality:

$$\mathrm{d}W/\mathrm{d}z \ll (\pi/\xi_h)^2. \tag{18}$$

In fact, condition (18) coincides with the condition of validity of the Eikonal approximation for X-rays, which was obtained by Authier & Balibar (1970). Hence, we can consider the Eikonal approximation of the X-ray dynamical theory as an analogy of the adiabatic invariance concept for mechanical systems. It should be observed here that the new interpretation of the X-ray interbranch scattering, which is expressed in terms of quantum mechanics, follows from it. Taking into account that the adiabatic analogy is not valid in the case of the X-ray interbranch scattering, we can consider this process as a beating transition one, which happens between close quantum levels in the case of the violation of adiabatic invariance. Moreover, we suppose that these levels are separated by a potential barrier as well. Then, the quantum transition taking place is due to the 'tunnel' effect. The description of such quantum systems can be found in detail in Landau & Lifshitz (1989). It should be recalled that Penning (1966) was the first who paid attention to the link between the X-ray interbranch scattering and the quantum 'tunnel' effect. We hope also that the proposed quantum model of X-ray interbranch scattering will be useful for a deeper insight into this problem.

4. Conclusions

Here we sum up the main results obtained in this work:

1. The generalized pendulum analogy of the X-ray dynamical diffraction was developed to describe the case of an off-Bragg position. A difference between the pendulum masses was introduced into consideration for this purpose. By introducing a time variation of these masses, it is possible also to simulate the X-ray diffraction by a 1D regularly deformed crystal.

2. We have established an analogy between the adiabatic invariants of the generalized pendulum model and the invariants of the X-ray Eikonal approximation. This means that a direct correspondence exists between the concept of adiabatic invariance in classical mechanics and the Eikonal approach of X-ray dynamical diffraction by a regularly deformed crystal.

3. Using the quantum mechanics analogy, which is based on the adiabatic invariant model, a new interpretation of the X-ray interbranch scattering process has been presented. It consists in the supposition that this process can be considered as a beating one.

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