SOLUTION OF UNSTEADY PROBLEM OF MECHANICAL VIBRATIONS OF ONE-DIMENSIONAL CHAIN OF ELASTICALLY COUPLED PARTICLES IN THE PRESENCE OF AN ISOBARIC DEFECT

V. V. Mazhuga

The one-dimensional chain of elastically coupled particles is the simplest model for studying the statistical dynamic properties of solid bodies. Schrödinger [1] obtained an analytic solution of the unsteady problem of uniform chain vibrations and examined the transition from the mechanics of a system of discrete points to the mechanics of a continuum.

The time dependence of the motion of a linear chain in the presence of an isotopic defect (the foreign particle differs only in mass from the basic particle) was studied in [2]. Using the generating function method, he obtained the integral equations of motion of the chain particles, which he solved by iterations, and then was able to sum the resulting series. In view of the complexity of the formulas, this method cannot be used in practice to examine unsteady problems of vibrations of a chain with other types of defects, e.g., the case of presence in the chain of an isobaric defect (the foreign particle differs from the basic particle only in its interaction with its neighbors), a molecular contaminant, and so on. In the present study we obtain the solution of the unsteady problem of vibrations of a chain in the presence of an isobaric defect.

1. We shall study the problem of longitudinal vibrations of an infinite chain consisting of particles of mass M arranged in a straight line and in a state of equilibrium at equal distances from one another. Particle interaction is examined in the harmonic approximation. We denote the chain force constant by K. In the chain one node (zero) is occupied by a particle whose interaction is described by the force constant K_0 and is different from the interaction between the remaining particles.

The system of equations describing the motion of the particles has the form

$$r_i^{\cdot\cdot}(t) = [K + (K_0 - K)(\delta_{i,0} + \delta_{i,-1})](r_{i+1} - r_i) - [K + (K_0 - K)(\delta_{i,0} + \delta_{i,1})](r_i - r_{i-1}) \quad (1.1)$$

where r_i ($i = 0, \pm 1, \pm 2, \ldots$) is the deviation of the i-th particle from the equilibrium position, and δ_{in} is the Kronecker symbol.

The initial conditions are

$$r_i(0) = a_i, \quad r_i^{\cdot}(0) = v_i \quad (1.2)$$

Introducing the dimensionless time τ, we obtain

$$4r_i^{\cdot\cdot}(\tau) = [1 + (\beta - 1)(\delta_{i,0} + \delta_{i,-1})](r_{i+1} - r_i) - [1 + (\beta - 1)(\delta_{i,0} + \delta_{i,1})](r_i - r_{i-1})$$
$$r_i(0) = a_i, \quad r_i^{\cdot}(0) = v / \omega_L \, (\tau = 2(K/M)^{1/2} t = \omega_L t, \quad \beta = K_0 / K) \quad (1.3)$$

The solution of this system of linear differential equations with constant coefficients can be sought in the form

$$r_i(\tau) = \sum_{j=-\infty}^{\infty} \left[a_j \Phi_i(j, \tau) + \frac{v}{\omega_L} \int_0^{\tau} \Phi_i(j, \tau')\, d\tau' \right] \quad (1.4)$$

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The problem reduces to finding the function $\Phi_i(j, \tau)$.

Thus, we shall solve (1.3) with the initial conditions

$$r_i(0) = a_i, \quad r_i^{\cdot}(0) = 0 \tag{1.5}$$

2. We solve the problem by the Laplace transform method. If we denote the transform of the function $r_i(\tau)$ by $x_i(p)$, it is not difficult to find

$$\begin{aligned}&[1 + (\beta - 1)(\delta_{i,0} + \delta_{i,-1})][x_{i+1}(p) - x_i(p)] \\ &- [1 + (\beta - 1)(\delta_{i,0} + \delta_{i,1})][x_i(p) - x_{i-1}(p)] - 4p^2 x_i(p) + 4pa_i = 0\end{aligned} \tag{2.1}$$

We examine (2.1) for i = 2, 3, 4, ...

$$x_{i+1} - (4p^2 + 2)x_i + x_{i-1} + 4pa_i = 0 \tag{2.2}$$

Equation (2.2) is a homogeneous difference equation and its solution is [3]

$$x_i = \varphi_1^{-1}\Big(\varphi_{i-1}x_2 - \varphi_{i-2}x_1 + 4p\sum_{\nu=2}^{i-1}\varphi_{\nu-1}a_{i+1-\nu}\Big), \quad \varphi_i = (\sqrt{p^2+1} + p)^{2i} - (\sqrt{p^2+1} - p)^{2i} \tag{2.3}$$

An analogous relation holds for x_i with negative values of the index i:

$$x_k = \varphi_1^{-1}\Big(\varphi_{-k-1}x_{-2} - \varphi_{-k-2}x_{-1} + 4p\sum_{\nu=-2}^{k+1}\varphi_{-\nu-1}a_{k-1-\nu}\Big) \tag{2.4}$$

Here negative values of the particle numbers are denoted by the index k.

Using (2.1) with t = −1, 0, 1 and (2.3), (2.4), after simple algebraic transformations we find

$$\begin{aligned}(4p^2 + 2\beta)x_0 &= \beta\sigma_{i-1}^{-1}\Big(\beta\varphi_{i-1}x_0 + \varphi_1 x_i + 4p\sum_{\nu=2}^{i}\varphi_{\nu-1}a_{i+1-\nu}\Big) \\ &+ \beta\sigma_{-k-1}^{-1}\Big(\beta\varphi_{-k-1}x_0 + \varphi_1 x_k + 4p\sum_{\nu=-2}^{k}\varphi_{-\nu-1}a_{k-1-\nu}\Big) + 4pa_0 \\ \sigma_i &= [(4p^2 + \beta + 1)\varphi_i - \varphi_{i-1}]\end{aligned} \tag{2.5}$$

Passing in (2.5) to the limit as $i \to \infty$ and $k \to -\infty$, we obtain $x_0(p)$

$$\begin{aligned}x_0(p) &= \frac{1}{\Delta}\Big[\beta\sum_{j=-\infty}^{\infty}(\sqrt{p^2+1} - p)^{2|j|}a_j + 2(1-\beta)p(\sqrt{p^2+1} - p)a_0\Big] \\ \Delta &= \beta\sqrt{p^2+1} + (\beta - 1)p[(\sqrt{p^2+1} - p)^2 - 1]\end{aligned} \tag{2.6}$$

Finding $r_0(\tau)$ reduces to calculating the contour integral

$$r_0(\tau) = \frac{1}{2\pi i}\int_{a-i\infty}^{a+i\infty} x_0(p)e^{p\tau}\,dp \tag{2.7}$$

where a is a constant which is larger than the real part of any singularity of $x_0(p)$.

The contour integral (2.7) can be expressed in terms of Lommel, Bessel, and trigonometric functions [4]. The Lommel functions of two independent variables are defined by the relation (see [5] for tables of the Lommel functions)

$$U_\nu(y, z) = \sum_{m=0}^{\infty}(-1)^m\Big(\frac{y}{z}\Big)^{\nu+2m}J_{\nu+2m}(z) \tag{2.8}$$

Replacing the variable in (2.7) using $w = p - \sqrt{p^2+1}$, we have

$$\begin{aligned}r_0(\tau) &= \frac{1}{2\pi i}\oint_l x_0(w)\exp\Big[\frac{\tau}{2}\Big(w - \frac{1}{w}\Big)\Big]dw \\ x_0(w) &= \frac{1 + w^2}{w[(3\beta - 2)w^2 + 1]}\Big\{\beta\sum_{j=-\infty}^{\infty}w^{2|j|}a_j + (\beta - 1)(w^2 - 1)a_0\Big\}\end{aligned} \tag{2.9}$$

We can take as the contour l any circle enclosing the coordinate origin $w=0$ and not enclosing the poles of the integrand. Here it is assumed that the coordinate origin is bypassed in the positive direction.

We represent the function $x_0(w)$ in the form of the sum of fractions:

$$x_0(w)=\frac{A_{00}}{w}+\sum_{n=1}^{\infty}\sum_{k=1}^{2}\frac{A_{nk}w^{2n+1}}{w^2-w_k}, \quad w_{1,2}=\frac{2-3\beta\pm\gamma}{2-2\beta}, \quad \gamma=(9\beta^2-8\beta)^{1/2} \tag{2.10}$$

The integral (2.9) breaks down into the sum of integrals of the form

$$I_1=\frac{1}{2\pi i}\int_l w^{-1}\exp\left[\frac{\tau}{2}\left(w-\frac{1}{w}\right)\right]dw \tag{2.11}$$

$$I_2=\frac{1}{2\pi i}\int_l \frac{w^{2n+1}}{w^2-w_k}\exp\left[\frac{\tau}{2}\left(w-\frac{1}{w}\right)\right]dw \tag{2.12}$$

The integral (2.11) is the Bessel function $J_0(\tau)$ of zero order [6].

Expanding the denominator in (2.12) into a series, it is easy to show that for $\beta<1$ the integral (2.12) equals

$$I_2=(-w_k)^n U_{2n+2}\left[\left(-\frac{1}{w_k}\right)^{1/2}\tau,\tau\right] \tag{2.13}$$

For $\beta>1$ we obtain

$$I_2=(-w_k)^n U_{-2n+2}[(-w_k)^{1/2}\tau,\tau]-w_k^n\cos\omega_0\tau, \quad \omega_0=\left(\frac{2\beta}{4-3\beta+\gamma}\right)^{1/2} \tag{2.14}$$

Calculating sequentially all the integrals, after simple algebraic transformations we obtain $r_0(\tau)$. We introduce the notations

$$\begin{gathered}A=\frac{\beta-\gamma}{\gamma}\delta_{j,0}+\frac{\beta(\alpha^2-1)}{\alpha^{2|j|-2|\theta(j)|+2}\gamma}(1-\delta_{j,0}), \quad \alpha=\left(-\frac{1}{w_1}\right)^{1/2}\\ B=\frac{\beta+\gamma}{\gamma}\delta_{j,0}+\frac{\beta(\delta^2-1)}{\delta^{2|j|-2|\theta(j)|+2}\gamma}(1-\delta_{j,0}), \quad \delta=\left(-\frac{1}{w_2}\right)^{1/2}\\ \theta(j)=1\ (j\geqslant 1), \quad \theta(j)=0\ (j=0), \quad \theta(j)=-1\ \ (j\leqslant 1)\end{gathered} \tag{2.15}$$

Then with account for (1.4) the solution can be written in the forms:

for $\beta>1$

$$\Phi_0(j,\tau)=J_0(\tau)\delta_{j,0}+(-1)^{|j|-\theta(j)|+1}A\cos\omega_0\tau+AU_{2|\theta(j)|-2|j|}(\alpha^{-1}\tau,\tau)-BU_{2|j|-2|\theta(j)|+2}(\delta\tau,\tau) \tag{2.16}$$

for $\beta<1$

$$\Phi_0(j,\tau)=J_0(\tau)\delta_{j,0}+AU_{2|j|-2|\theta(j)|+2}(\alpha\tau,\tau)-BU_{2|j|-2|\theta(j)|+2}(\delta\tau,\tau) \tag{2.17}$$

For the case $\beta=1$ the solution was obtained previously in [1].

Now we turn to finding $r_i(\tau)$ for $i\neq 0$. Substituting x_2 from (2.3) into (2.1) for $i=1$, and x_{-2} from (2.4) into (2.1) for $i=-1$, we have

$$x_1=\sigma_{i-1}^{-1}\left(\beta\varphi_{i-1}x_0+\varphi_1 x_i+4p\sum_{\nu=2}^{i}\varphi_{\nu-1}a_{i+1-\nu}\right) \tag{2.18}$$

$$x_{-1}=\sigma_{-k-1}^{-1}\left(\beta\varphi_{-k+1}x_0+\varphi_1 x_k+4p\sum_{\nu=-2}^{k}\varphi_{-\nu-1}a_{k-1-\nu}\right) \tag{2.19}$$

Subtracting (2.19) from (2.18) and passing to the limit as $i\to\infty$ and $k\to-\infty$, we obtain

$$x_1(p)-x_{-1}(p)=\frac{4p}{1+(\beta-1)(\sqrt{p^2+1}-p)^2}\sum_{j=-\infty}^{\infty}\theta(j)(\sqrt{p^2+1}-p)^{2|j|}a_j \tag{2.20}$$

Using the equation of (2.1) for $i=0$ and (2.20), we find the transforms $x_1(p)$ and $x_{-1}(p)$, and then from (2.18) and (2.19) we obtain $x_i(p)$ and $x_k(p)$.

We find the original by the method used for finding the original of $x_0(p)$. We present the final result, using the notation (1.4).

If $\beta > 2$, then

$$\Phi_i(j,\tau) = \Psi_i(j,\tau) + (-1)^{|i|+|j|} C \cos \omega_0\tau + (-1)^{|i|+|j|} E\theta(i)\theta(j)\cos\omega_1\tau + CU_{2-2|i|-2|j|}(\alpha^{-1}\tau, \tau) + E\theta(i)\theta(j)U_{2-2|i|-2|j|}(\varepsilon^{-1}\tau, \tau) \qquad (2.21)$$

Here

$$\Psi_i(j,\tau) = J_{2|i-j|}(\tau) - J_{2|i|+|2j-\theta(j)|-2}(\tau) + \frac{1}{2}[1-\delta_{j,0}+\theta(i)\theta(j)][(1-\beta)J_{2|i|+2|j|-2}(\tau) + J_{2|i|+2|j|-4}(\tau)] + DU_{2|i|+2|j|}(\delta\tau, \tau) \qquad (2.22)$$

$$C = \frac{\beta(\alpha^2-1)}{\alpha^{2|i|}\gamma}\delta_{j,0} + \frac{2\beta^2-3\beta^3-\beta^2\gamma+2\beta\gamma}{4\alpha^{2|i|+2|j|-2}\gamma(1-\beta)}(1-\delta_{j,0})$$

$$D = \frac{\beta(1-\delta^2)}{\delta^{2|i|}\gamma}\delta_{j,0} + \frac{3\beta^3-2\beta^2-\beta^2\gamma+2\beta\gamma}{4\delta^{2|i|+2|j|-2}\gamma(1-\beta)}(1-\delta_{j,0})$$

$$E = \frac{\beta^2-2\beta}{2(\beta-1)^{|i|+|j|}}, \quad \varepsilon = (\beta-1)^{1/2}, \quad \omega_1 = \frac{\beta}{2\sqrt{\beta-1}}$$

For $1 < \beta \leq 2$ the solution has the form

$$\Phi_i(j,\tau) = \Psi_i(j,\tau) + (-1)^{|i|+|j|} C\cos\omega_0\tau + CU_{2-2|i|-2|j|}(\alpha^{-1}\tau, \tau) + E\theta(i)\theta(j)U_{2|i|+2|j|}(\varepsilon\tau, \tau) \qquad (2.23)$$

In the case $\beta < 1$ we find

$$\Phi_i(j,\tau) = \Psi_i(j,\tau) + CU_{2|i|+2|j|}(\alpha\tau, \tau) + E\theta(i)\theta(j)U_{2|i|+2|j|}(\varepsilon\tau, \tau) \qquad (2.24)$$

For $\beta = 1$ the solution was obtained in [1].

3. Example. We shall investigate the statistical dynamic properties of a chain with isobaric defect. Assume that at the initial time $t = 0$ the velocity of the i-th particle has the given value $v_i(0)$, and the velocities of the remaining particles are random quantities with canonical distribution. We examine the establishment of Maxwellian distribution in the given chain. In order to study the approach to the equilibrium velocity of an individual chain particle, we must find the conditional probability distribution of the velocity of this particle, defined by the relation

$$P[v_i(t)\,|\,v_i(0)] = \frac{W_2[v_i(t)\,|\,v_i(0)]}{W_1(v_i)} \qquad (3.1)$$

Here $W_1(v_i)$ denotes the probability density for the value v_i to fall in the interval v_i, $v_i + dv_i$; $W_2[v_i(t)\,|\,v_i(0)]$ denotes the joint probability density for the value of v_i to fall in the interval $v_i(t)$, $v_i(t) + dv_i(t)$ at the time t and the interval $v_i(0)$, $v_i(0) + dv_i(0)$ at the time 0. It can be shown [2] that $P[v_i(t)]v_i(0)]$ has the form

$$P[v_i(t)\,|\,v_i(0)] = \{2\pi\langle v_i^2\rangle[1-\Phi_i^2(i,t)]\}^{-1/2} \exp\left\{-\frac{[v_i(t)-\Phi_i(i,t)v_i(0)]^2}{2\langle v_i^2\rangle[1-\Phi_i(i,t)]}\right\} \qquad (3.2)$$

Here the angle brackets denote canonical ensemble averaging.

It follows from (3.2) that the behavior of $P[v_i(t)\,|\,v_i(0)]$ is determined by the behavior of $\Phi_i(i, t)$. It is not difficult to show that in the formulas obtained for $\Phi_i(i, \tau)$ (we note that $\tau = \omega_L t$), all the terms approach zero as $\tau \to \infty$, except the terms containing the cosine. These terms correspond to local vibrations. Consequently, the Maxwellian distribution is established in the system only for $\beta \leq 1$. In the remaining cases the conditional probability distribution function does not approach the Maxwellian distribution but depends on the initial quantity $v_i(0)$ and has a periodic nature.

Thus, in the harmonic approximation in the presence of local vibrations in the chain there is not equipartition of the energy among all the particles. A similar result was obtained in [2] for a chain with isotopic defect.

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