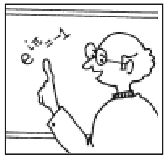
Classroom



In this section of *Resonance*, we invite readers to pose questions likely to be raised in a classroom situation. We may suggest strategies for dealing with them, or invite responses, or both. “Classroom” is equally a forum for raising broader issues and sharing personal experiences and viewpoints on matters related to teaching and learning science.

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The Discrete, the Continuous and the ‘Concrete’ Classical Harmonic Dynamics

An elementary treatment of the classical harmonic dynamics of a linear (1D) array of identical point-like masses (particles) with equal couplings (elastic spring constants) is re-considered in three distinct limits – the Discrete, where the mass-points are identical and equispaced while the elastic springs are massless; the Continuous, where we have a 1D elastic medium of uniform mass-density (mass per unit length); and the ‘Concrete’ lattice which comprises an elastic 1D continuum having a uniform mass-density *and* is embedded in the identically coupled equispaced mass-points. Analytical expressions are obtained for some elementary, but often rather subtle, quantities of physical interest, e.g., the mechanical power transported, and the mechanical momentum associated with such an apparently simple purely oscillatory 1D harmonic lattice system. The classroom exercise will conclude with a suggestion for the possibility that the ‘Concrete’ case may well correspond to that of hard nanoparticulate crystallites embedded in a 1D elastic continuum, e.g., a spider dragline silk, known for

Keywords
Discrete, continuous, concrete, 1D classical lattice dynamics, 1D transport momentum, velocity, power.

its exceptionally fast vibrational-energy transport, which is in fact comparable to that of diamond! This should hopefully provide a motivating thought for the curious among the young readers of *Resonance*.

1. Introduction: The Physical Problem

It is well known that an inertial mass (m), disturbed weakly from its state of classical-mechanical equilibrium (the ground state), will perform a phased oscillatory motion of small amplitude about its equilibrium position. This undamped oscillation describes its harmonic dynamics. Such a motion is characterized generally by a coupling constant k (stiffness), a circular frequency ω corresponding to its time period ($T = 2\pi/\omega$), and an amplitude A (real) of its oscillations. This in turn determines the associated oscillator energy (kinetic K and potential U), with the total energy ($K + U$) remaining constant in time – a conserved quantity for the dynamical system (without any friction). This simple harmonic oscillator model can be extended to a rich class of dynamical systems, now subsumed under Lattice Dynamics – a fascinating chapter in classical solid state physics. The purpose of this Classroom exercise is to introduce certain basic ideas of lattice dynamics with a minimum of jargon. We will in particular define and describe three distinct cases that may conveniently be named as the Discrete ('Dis-crete'), the Continuous ('Con-tinuous'), and somewhat unconventionally, as the 'Concrete' ('Con-crete')! A central, rather subtle issue will be to resolve as to if, and when such a purely oscillatory mechanical-wave motion can transport power (energy transported per unit time) across an arbitrarily chosen lattice point/site, n say, and have a linear mechanical momentum associated with it.

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2. The Discrete Case

Let us begin with the discrete case of a 1D N-site

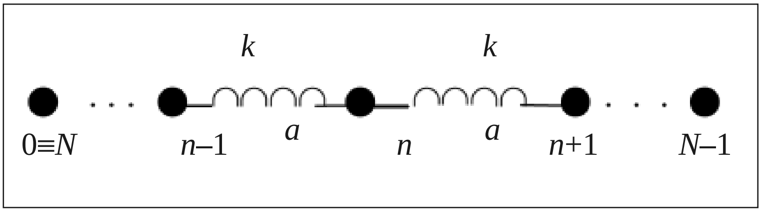

Figure 1. 1D N-site lattice of total mass Nm coupled by massless harmonic springs, of spring constant 'k' with spring length (lattice constant) 'a', and subjected to the periodic boundary condition, i.e., site N is identified with a site 0, making it effectively a closed string of coupled mass-points. Let $N \gg 1$ (essentially infinite) so that the mass-point motion is almost tangential to the closed string, though this is really not necessary. We will be considering only the longitudinal motion of the mass-points.

harmonic lattice of equal point-masses coupled by identical nearest-neighbour springs of relaxed length (lattice constant) 'a', as indicated in *Figure* 1

It should be noted that the lattice points here merely label the points/sites on the x-axis, say, when the coupled mass-points are in the ground state – *the mass-points are not physically pinned on any rigid substrate.* Also, while the particles carry mass (i.e., they are *mass-points*), the inter-particle elastic couplings (springs) are massless – and hence the interactions between the neighbouring mass-points are instantaneous, i.e., there is no time delay involved here.

The simple harmonic equation of motion for the lattice system then becomes

$$m\frac{\mathrm{d}^2u_n(t)}{\mathrm{d}t^2} = -k(2u_n(t) - u_{n+1}(t) - u_{n-1}(t)), \qquad (1)$$

where $u_n(t)$ is the displacement of the nth mass-point from its initial (equilibrium) position at site n; m is its mass; and k is the spring constant coupling the nearest-neighbours. (Note that we will often write just u_n for $u_n(t)$ when there is no possibility of confusion).

Equation (1) follows simply from the well-known classical mechanical Lagrangian

$$L \equiv K - U \equiv \sum_n \frac{1}{2}m\left(\frac{\mathrm{d}u_n(t)}{\mathrm{d}t}\right)^2 - \sum_n \frac{1}{2}k(u_n(t) - u_{n-1}(t))^2, \qquad (2)$$

where K is the total kinetic energy and U is the total potential energy for the harmonically coupled system. The corresponding Lagrangian equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{u}_n}\right) - \frac{\partial L}{\partial u_n} = 0, \qquad (3)$$

then gives at once our *equation of motion* (1) as displayed above. The overhead dot in $\dot{u}_n$ denotes the time derivative.

Section 2 is basically concerned with this somewhat subtle effect of there being a non-zero translatory displacive velocity of the centre-of-mass for an apparently purely oscillatory simple-harmonic motion of mass-points of the effectively infinite lattice above!

Here one is tempted to conclude that the *total mechanical momentum* carried by our N-site periodic system must add up to *zero* inasmuch as every mass-point executes a phased classical simple-harmonic motion which is periodic in time and the lattice space. But, as we will presently show, this is *not* the case in general – indeed, there is a net *mechanical momentum* carried by the uniform motion of the *centre-of-mass* of the whole dynamical system, over and above the purely oscillatory motion naturally expected otherwise. Section 2 is basically concerned with this somewhat subtle effect of there being a non-zero translatory displacive velocity of the centre-of-mass for an apparently purely oscillatory simple-harmonic motion of mass-points of the effectively infinite lattice above!

In order to clearly see that this indeed is the case, we have to solve our starting linear differential equation (1). To this end, let us apply an impulsive force $= I\delta_{n0}\delta(t)$ at site $n = 0$, directed to the right, say. (Here, I is the total impulse applied). Now, introduce the time-Laplace transform

$$\mathcal{L}u_n(t) \equiv \int_0^\infty e^{-st} u_n(t)\mathrm{d}t \equiv \tilde{u}_n(s), \qquad (4)$$

together with the spatial Lattice (discrete) Fourier transform

$$\mathcal{F}u_n(t) \equiv \sum_0^{N-1} u_n(t)e^{iqn} \equiv \bar{u}_q(t) \qquad (5)$$

and solve quite straightforwardly the resulting algebraic equation for $\mathcal{LF}(u_n(t)) \equiv \bar{\tilde{u}}_q\,(s)$, giving

$$\mathcal{LF}(u_n(t)) = \frac{I}{m(s^2 + 4\omega^2 \sin^2 q/2)} \equiv \bar{\tilde{u}}_q\,(s), \qquad (6)$$

where I in the numerator is the impulse applied at the left end of the periodic lattice $0 \leq n \leq N-1$, and $\omega \equiv \sqrt{k/m}$. The notations $\mathcal{L}, \mathcal{F}$, and $\mathcal{LF}$, respectively, denote the Laplace, the Fourier, and the Laplace-Fourier transforms. The overhead symbol $\simeq$ denotes $\mathcal{LF}(u_n(t))$. This notation is obvious from the context above. Here, we have used the initial-value theorem for the Laplace transform of time-derivative of the wave amplitude $u_n(t)$, namely, $\mathcal{L}\dot{u}_n(t) = s\tilde{u}_n(s) - u_n(0)$. Also, the variable q is the usual wavevector with $-\pi/a \leq q \leq \pi/a$ for the periodic boundary condition assumed here. The lattice constant a will be set equal to unity.

Now, the Laplace-Fourier transform in (6) is readily inverted to yield

$$u_n(t) = \frac{1}{N}\sum_q \left(\frac{I}{2m\omega \sin q/2}\right)(\sin(2\omega t \sin q/2))e^{-iqn}, \qquad (7)$$

giving the quantity of interest, namely the total mechanical momentum

$$\begin{aligned} & m\sum_0^{N-1} \dot{u}_n(t) \\ & = \frac{m}{N}\sum_n \left(\frac{I}{2m\omega \sin q/2}\right)\sin(2\omega t \sin q/2)e^{-iqn} \\ & \equiv I \end{aligned} \qquad (8)$$

Under an impulsive force, a discrete 1D classical harmonic lattice of mass-points with mass-less elastic couplings can deive a persistent displacive velocity for periodic boundary conditions.

for the given impulse $I(>0)$ applied rightward on the lattice.

Thus, our final solution implies that the lattice as a whole is being displaced (it *slides*) at a constant rightward velocity $V_0 = I/Nm$ in response to the impulse I.

There is *no* net mechanical momentum associated with the *sinusoidally oscillating harmonic lattice*!

In order to fully appreciate this point, consider a lattice system of just two mass-points ('beads') as having been kicked by an impulsive force (of impulse I) applied rightward at the first mass-point. (The kick may be imparted, e.g., by a speeding nucleus!). This problem has the well-known elementary solution – namely, a uniformly displacive (translating) centre-of-mass velocity, and an oscillatory relative motion of the two mass-points about their centre-of-mass, and thus *carrying no net mechanical momentum by themselves.* (Incidentally, this oscillatory motion is what is referred to as the '*normal mode*'.

In order to fully appreciate this point, consider a lattice system of just two mass-points (`beads') as having been kicked by an impulsive force (of impulse I) applied rightward at the first mass-point.

Next, one may ask a related question of some physical interest, namely how a discrete infinitely long harmonic lattice with the periodic sinusoidal motion can at all transport a *net non-zero mechanical power*? The answer to this question, however, turns out to be quite straightforward. Here, for the discrete lattice dynamics described by equation (1), the mechanical power (energy transported per unit time) at time t *across a site*, n say, towards its right is given by

$$P_n(t) = k(u_{n-1}(t) - u_n(t)) \times \text{the velocity } \left(\frac{\partial \mathrm{u_n(t)}}{\partial \mathrm{t}}\right). \tag{9a}$$

Now, for the running sinusoidal wave in question here, we have the displacement $u_n(t) = A\sin(\Omega t - n\phi)$, where $u_n(t)$ satisfies the equation following from (1), namely

$$\begin{aligned} -m\Omega^2 A\cos(\Omega t - n\phi) &= -kA[2\cos(\Omega t - n\phi) \\ &\quad - \cos(\Omega t - (n+1)\phi) - \cos(\Omega t - (n-1)\phi), \end{aligned} \tag{9b}$$

A discrete 1D harmonic periodic lattice of mass-points with massless elastic couplings can transport mechanical power across an arbitrarily chosen lattiice point, without transporting matter through the system.

where $\sqrt{k/m} = \omega$ is the circular frequency for the spring constant k and the point-mass m, and $\phi =$ the phase advance over a lattice spacing (lattice constant 'a'), chosen to be unity here. The associated wave-mode frequency

Ω is readily determined from (9b) as

$$\Omega = 2\omega \mid \sin\phi/2 \mid . \tag{9c}$$

All one has to do now is to substitute (9b) and (9c) in the basic (9a), obtaining

$$\begin{aligned} \langle P_n(t)\rangle &= -A^2\Omega\langle[\cos(\Omega t-(n-1)\phi)-\cos(\Omega t-n\phi)] \\ &\qquad \times \sin(\Omega t-n\phi)\rangle \\ &= -A^2\Omega\langle[\cos(\Omega t-n\phi)\cos\phi-\sin(\Omega t-n\phi)\sin\phi \\ &\qquad -\cos(\Omega t-n\phi)]\times\sin(\Omega t-n\phi)\rangle \\ &= A^2\omega \mid \sin\phi/2 \mid \times\sin\phi\neq 0, \text{in general,} \end{aligned} \tag{10}$$

where we have made use of the orthogonality $\langle\cos(\Omega t - n\phi)\cdot\sin(\Omega t-n\phi)\rangle = 0$, and the normalization $\langle\sin^2(\Omega t - n\phi)\rangle = 1/2$ for the time-average. Also, we have substituted for Ω from (9c). Following convention, we may write for the phase advance (per lattice constant) $\phi \equiv qa$, with $-\pi \leq qa \leq \pi$ being the familiar first-Brillouin zone (I-BZ), with the zone boundary $\pm\pi$ for the 1D system considered here.

Hence, there is indeed a non-zero time-averaged mechanical power transported across any site 'n' on the infinite 1D lattice. For the wavevector q greater/less than zero, the wave clearly propagates to the right/left. The power transport is readily seen to vanish, both at $qa = 0$ and $qa = \pm\pi$, the I-BZ boundaries. Equation (10) is one of the main results of Section 1.

We now turn to the case of the continuous 1D elastic medium with a uniformly distributed mass-density per unit length. The question now is, if and how can such a 1D system transport non-zero power and mechanical momentum. Again, only the longitudinal displacement waves will be considered. (It may be recalled that for an infinitely long 1D system, boundary conditions essentially become irrelevant. Indeed, one may always resort to the periodic boundary condition, or effectively, concentrate only on the region far from the distant ends of the 1D system).

3. The Continuous Case

This is rather subtle. The harmonic motion of a 1D elastic medium may, of course, be expected to give the well-known wave equation

$$\frac{\partial^2 u(x,t)}{\partial t^2} = v^2 \frac{\partial^2 u(x,t)}{\partial x^2}, \tag{11}$$

where $u(x,t)$ is the longitudinal displacement at the space-time point (x,t), and v is the velocity of the wave along the x-axis with $v^2 = Y/\mu$. Here Y is Young's modulus (= force/extension) and μ is the linear mass density (i.e., mass per unit length).

Wave equation (11) follows readily from the Lagrangian density $\mathcal{L}$ for the 1D elastic medium

$$\mathcal{L} = \frac{1}{2}\left[\mu\left(\frac{\mathrm{d}u(x,t)}{\mathrm{d}t}\right)^2 - Y\left(\frac{\mathrm{d}u(x,t)}{\mathrm{d}x}\right)^2\right] \tag{12}$$

and the associated Lagrangian equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial\mathcal{L}}{\partial\left(\frac{\mathrm{d}u(x,t)}{\mathrm{d}t}\right)}\right) + \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial\mathcal{L}}{\partial\left(\frac{\mathrm{d}u(x,t)}{\mathrm{d}x}\right)}\right) = 0, \tag{13}$$

giving the linear equation (4) with a sinusoidal running-wave solution

$$u(x,t) = A\sin q(x - vt). \tag{14}$$

This equation is often also re-written as $u(x,t) = A\sin(qx - \Omega t)$, where Ω is the circular frequency corresponding to the wavevector q. Here, A is the wave amplitude, and it is real. Clearly, $v > 0$ implies a wave propagating in the positive x-direction.

A 1D elastic medium of finite mass per unit length (linear density) can sustain a longitudinal wave motion, without transporting matter and energy through the system.

Following are some of the notable features of this longitudinal wave motion in the 1D elastic continuum. It causes locally an oscillatory longitudinal displacement. The phase $(\Omega t - qx)$ of the wave varies linearly in x

There is a fundamental difference between the discrete and the continuous 1D systems. Implicit in the discrete lattice dynamics is the assumption that the displacement amplitude is always smaller than the lattice spacing '*a*'.

and t. Associated with this, there are periodic fluctuations in the local mass-density (per unit length) *without* transport of matter or mechanical momentum over any finite distance. Here we have, however, a fluctuation of the energy density (kinetic as well as potential) which is periodic in space–time.

Very importantly, there is *no* transport of mechanical energy associated with this wave – hence often referred to as a phase-wave. One may attempt to draw an analogy with our earlier treatment following equation (9c) for the discrete-lattice case *in the limit of the lattice constant 'a' tending to zero*. This is, however, misleading. There is a fundamental difference between the discrete and the continuous 1D systems. Implicit in the discrete lattice dynamics is the assumption that the displacement amplitude is always smaller than the lattice spacing 'a'. (Of course, the mass-points are not pinned to the lattice sites). This is clearly violated in the case of the continuum. Thus, equation (9c) for the discrete lattice case becomes *invalid* in the case of the continuum considered in the present section.

As an aside, one may, however, consider the case of a *1D gaseous systems*, e.g., a gas of molecules confined in an infinitely long but *very narrow* tube, allowing almost free motion along the tube. This can, e.g., sustain a longitudinal sound wave of roughly 1D character. But then, this is a different system altogether, and we will not consider it any further.

4. The 'Concrete' (Continuous-Discrete) Case

Finally, we turn to the Continuous-Discrete ('Concrete') case. Here the continuous *elastic* 1D medium providing the inter-particle restoring force (stiffness) has a uniform *non-zero* mass density (mass per unit length), and the periodically distributed discrete point-like particles (mass-points) embedded in this elastic continuum too carry non-zero mass. This poses a relatively hard problem, compared to the one considered earlier in Section 1. There, the mass-less elastic spring exerted instantaneously-acting restoring force on the nearest-neighbouring mass-points. Here, in sharp contrast to that, the interaction between the two neighbouring mass-points is *mediated* by a wave propagating at a finite speed along the intervening elastic medium having non-zero mass per unit length. (In fact, the boundaries between the neighbouring mass-points and the intervening elastic medium *also* move). Such a system of mass-points coupled through the elastic 'mass-full' medium is qualitatively different from the cases discussed earlier. The problem is, however, well posed. It is indeed challenging. Here, however, we shall not attempt to solve this problem – it is posed here as an interesting Classroom exercise for the students. By way of added motivation, however, we would merely like to point out here a physically realizable analogue of this problem which is of considerable current scientific interest, namely that of a certain spider dragline silk with hard nanoparticulate crystallites embedded in the elastic fibre. This so-called dragline silk acts here as the elastic 1D medium, while the nanoparticulate crystallites act as the mass-points embedded periodically in it. This 'concrete' harmonic system can be readily modelled in terms of the usual three basic parameters – the linear mass density (mass per unit length) of the elastic dragline silk, its elastic constant (Young's modulus), and the mean spacing between the neighbouring mass-points (the crystallites here).

A nanoparticulate system of 1D periodic lattice off mass-points with nearest-neighbour couplings through an elastic medium of non-zero mass per unit length can transport energy, without transporting matter. The spider drafline silk would be a notable example.

This spider dragline silk is well known to exhibit some extraordinary physical properties, e.g., its vibrational-energy transport (lattice thermal conductivity) turns out to be comparable to that of diamond, and may in fact even exceed it! This, therefore, seems to be a remarkable example of a 'concrete' conductor. Admittedly, the real spider dragline silk is a highly complex

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material system of biomolecules (protein super-fibres). But, given the relative simplicity of the physical model as indicated above, mathematically inclined students of *Resonance* may be reasonably encouraged to pursue this problem in the overall spirit of a challenging Classroom exercise.

Suggested Reading

[1] Charles Kittel, *Introduction to Solid State Physics*, Fifth Edition, Wiley-Eastern Limited, New Delhi, 1977.

[2] L Brillouin, *Wave Propagation in Periodic Structures*, Dover, Phoenix Editions, 2003.

[3] Xiaopeng Huang, Guoqing Liu and Xinwei Wang, New Secrets of Spider Silk: Exceptionally High Thermal Conductivity and its Abnormal Change under Stretching, *Adv. Mater.*, Vol.24, pp.1482–1486, 2012.