

Evolution of a vibrational wave packet on a disordered chain

Philip B. Allen

Department of Physics and Astronomy, State University of New York, Stony Brook, New York 11794-3800

Jonathan Kelner

The Wheatley School, 11 Bacon Road, Old Westbury, New York 11568

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A linear chain of point masses coupled by harmonic springs is a standard model used to introduce concepts of solid state physics. The well-ordered chain has sinusoidal standing wave normal modes (if the ends are fixed) or traveling wave normal modes (if the ends are connected in a ring). Ballistically propagating wave packets can be built from these normal modes, and illustrate the mechanism of heat propagation in insulating crystals. When the chain is disordered, new effects arise. Ballistic propagation is replaced by diffusive propagation on length scales larger than the mean free path for ballistic motion. However, a new length scale, the localization length, also enters. On length scales longer than the localization length, neither ballistic nor diffusive propagation occurs, and energy is trapped unless there are anharmonic forces. These ideas are illustrated by a computer experiment. © 1998 American Association of Physics Teachers.

I. LINEAR CHAIN

Figure 1 shows a chain of point masses connected with springs. The n th mass has a nominal “equilibrium” position

na , where n is an integer, and a displacement u_n from the nominal position. Denoting the spring between mass n and mass $n+1$ as k_n , the potential energy of the system is

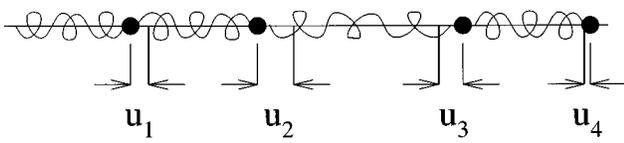


Fig. 1. A chain of point masses, showing the nominal positions—denoted by thick vertical lines, the actual positions, and the displacements u_n .

$$V = \frac{1}{2} \sum_{n=1} k_n (u_n - u_{n+1})^2 \quad (1)$$

since the springs are assumed to have unstretched length a equal to the spacing of the nominal positions. Newton's laws read

$$M_n \frac{d^2 u_n}{dt^2} = - \frac{\partial V}{\partial u_n}. \quad (2)$$

This paper is concerned with the question of how vibrational energy moves in time on such a chain.

All solutions of Newton's laws can be written as superpositions of the "normal modes" of vibration. These are the special solutions of Eq. (2) where every displacement $u_n(t)$ has the same time dependence, $u_n(t) = A u_{n\mu} \cos(\omega_\mu t + \phi)$. The index μ "counts" the normal modes, which are equal in number to the number of masses (or "atoms") on the chain. The pattern of displacements is given by the "eigenvector" $u_{n\mu}$, and the time dependence $\cos(\omega_\mu t + \phi)$ is independent of the "atom index" n . The amplitude and phase A and ϕ are free parameters to be fitted to initial data or chosen at will. When the chain is infinite and the springs k_n and masses M_n are all identical, the normal modes have the form $u_{n\mu} = \cos(Q_\mu n a)$ or $u_{n\mu} = \sin(Q_\mu n a)$. The wave vectors Q_μ are chosen to obey the boundary conditions on the chain; the infinite chain is mimicked by a finite chain of N "atoms" with periodic boundary conditions, and $Q_\mu = 2\pi\mu/Na$ obeys the requirements if μ is an integer. Only N distinct patterns $u_{n\mu} = \cos(Q_\mu n a)$ or $u_{n\mu} = \sin(Q_\mu n a)$ exist, and they can be chosen to be all the cosines and sines for integers μ from 0 to $N/2$. The subscript μ is superfluous because the value of Q is an equally good label. The cosine and sine solutions have the same frequency, which turns out to be

$$\omega_Q = 2\sqrt{k/M} \sin(Qa/2),$$

as derived in elementary solid state texts.¹ A particularly useful superposition state is the traveling wave

$$u_n(t) = |A_Q| \cos(Qna \pm \omega_Q t + \phi_Q). \quad (3)$$

$|A_Q|$ and ϕ_Q are free parameters. These states, after quantization, have energy $\hbar\omega_Q$ and are called "phonons." The model can be generalized to three-dimensional lattices and vector displacements \mathbf{u}_n . The resulting "phonon gas" picture is one of the basic building blocks of the physics of crystalline solids.

II. LOCALIZATION

This article is about some of the interesting changes that occur in the vibrations when the system is not perfectly ordered, but contains some random disorder. For simplicity the article considers one dimension and the case where the

masses are all the same but the springs have values $k + \delta k_n$, where δk_n is a small random number. A fundamental and surprising result is that for an infinite chain, disorder not only destroys the traveling wave nature of the normal modes of vibration, but it also causes the normal modes to be exponentially localized in space.² This means that beyond a sufficient distance from the "center" R_μ of the μ th normal mode, the amplitude of vibration decays exponentially with distance,

$$u_n \propto \exp(-|na - R_\mu|/\xi_\mu), \quad (4)$$

where the "localization length" ξ_μ is a property of the μ th normal mode. This phenomenon was first recognized by Anderson, and is referred to as "Anderson localization." The Nobel prize in 1977 was shared by Van Vleck, Mott, and Anderson. Anderson's citation³ referred specifically to his work on localization, and Mott's⁴ referred to his subsequent contributions to the same subject. A good recent reference is the book by Sheng.⁵ Thouless⁶ has written a good review of earlier work. There are two previous articles in *AJP* on localization on a chain,^{7,8} and a large literature of articles and reviews on the properties of eigenstates of chains.^{9,10}

Localization was first discussed as a property of a quantum electron in a disordered medium. A quantum electron behaves much like a classical wave. The results of localization theory therefore translate into consequences for classical waves. The connection between the Newtonian equation of motion for vibrations on a chain and the Schrödinger equation for a particle free to move on a chain of atoms is discussed in Appendix C.

III. WAVE PACKETS

Our concern will be the long-time behavior of a vibrational disturbance (a superposition of normal modes) which is initially spatially localized. A familiar example is a wave packet on a perfect chain. It is convenient to use complex numbers to represent the traveling wave solution, Eq. (3),

$$u_n(t) = A_Q e^{i(Qna - \omega_Q t)}. \quad (5)$$

Here A_Q is a complex number, related to the amplitude and phase in Eq. (3) as $A_Q = |A_Q| \exp(i\phi_Q)$. As usual, it is implied that the physical disturbance is the *real* part of this complex function. One advantage is that now the time dependence of $u_n(t)$ appears as a multiplicative factor $\exp(-i\omega_Q t)$, independent of n , so that the traveling wave solutions can be regarded as "normal modes" rather than superpositions.

The most general solution of Newton's laws is a superposition of traveling waves, with arbitrary complex coefficients A_Q ,

$$u_n(t) = \frac{1}{\sqrt{2\pi}} \int_{-\pi/a}^{\pi/a} dQ A_Q e^{i(Qna - \omega_Q t)}. \quad (6)$$

Here the sum over discrete wave vectors $Q = 2\pi\mu/Na$ is written as an integral over a continuous set, because the spacing $2\pi/Na$ goes to zero for a long chain. A wave packet is a spatially localized version of a traveling wave. The most convenient representation is to let the amplitude A_Q peak at a chosen wave vector Q_0 , and fall off with a Gaussian form,

$$A_Q = A e^{-iQR_0} e^{-(1/2)b^2(Q-Q_0)^2}. \quad (7)$$

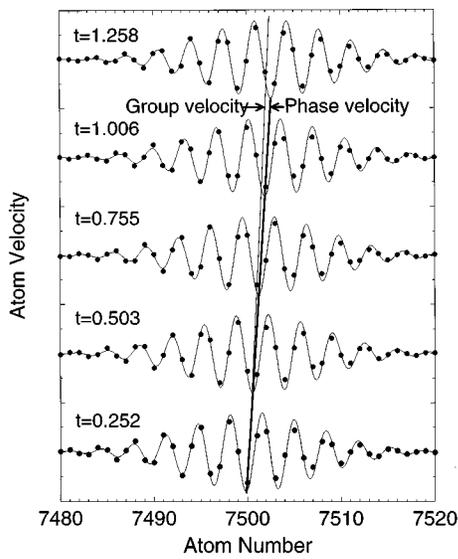


Fig. 2. The wave packet for short times. Time is measured in units of the period of the shortest vibration the chain can sustain. Distance is measured in units of the mass separation a . The solid line is Eq. (8). The dots are the actual positions of the point masses, with displacement plotted vertically for clarity. The calculations are made for a chain of length $15\,000a$, with R_0 chosen to be $7500a$, $Q_0=1.8235/a$, and $b=\sqrt{50}a$. The frequency ω_0 is 79% of the maximum frequency of the chain. The normal mode Q_0 has phase velocity $\omega_0/Q_0=2.72$ and group velocity $v_0=1.92$. These are indicated by sloping straight lines which denote the translation in time of a point of constant phase and of the center of energy, respectively. One complete period $2\pi/\omega_0=1.26$ is shown.

The phase factor $\exp(-iQR_0)$ has the effect of making the wave packet spatially centered at time zero on the “atom” at the location $na=R_0$. An explicit form for $u_n(t)$ can be found if the spread $1/b$ of wave vectors is small enough that the frequency ω_Q can be approximated by a Taylor series around the central frequency ω_0 (equal to ω_Q evaluated at $Q=Q_0$.) Similarly, the limits of the integral should safely extend to $\pm\infty$ because the contribution from $|Q|>\pi/a$ should be negligible. Denote the Taylor expansion by $\omega_Q \approx \omega_0 + v_0(Q-Q_0) + a_0(Q-Q_0)^2/2$, where v_0 is the group velocity $d\omega_Q/dQ$ and a_0 is the second derivative $d^2\omega_Q/dQ^2$. Then the integral in Eq. (6) is performed by completing the square in the exponent. The answer is

$$u_n(t) = \frac{A}{(b^2 + ia_0t)^{1/2}} \times \exp\left(-\frac{(na - R_0 - v_0t)^2}{2(b^2 + ia_0t)}\right) e^{i(Q_0na - \omega_0t)}. \quad (8)$$

This is a pulse centered at $R_0 + v_0t$ with a wave vector Q_0 , propagating ballistically with velocity v_0 . As shown in Appendix C, the energy is related to the squared modulus of this wave,

$$|u_n(t)|^2 = \frac{A^2}{(b^4 + a_0^2t^2)^{1/2}} \exp\left(-\frac{(na - R_0 - v_0t)^2}{(b^4 + a_0^2t^2)/b^2}\right). \quad (9)$$

The center of this pulse is at position $R_0 + v_0t$ for all times t . The spatial width of this pulse is $\sqrt{(b^2 + a_0^2t^2)/b^2}$, which equals b for short times. At longer times, the pulse spreads in width. This happens because the different normal mode com-

Table I. Modes of time evolution of a packet.

| | Center of pulse | Squared width of pulse |
|-------------|-----------------|------------------------|
| propagating | $R_0 + vt$ | $b^2 + a_0^2t^2/b^2$ |
| diffusing | R_0 | $b^2 + 2Dt$ |
| localized | R_0 | ξ^2 |

ponents propagate at slightly different group velocities $v_Q = v_0 + a_0(Q-Q_0)$. The width increases quadratically with time for intermediate times and linearly with time for large times.

Figure 2 shows such a Gaussian wave packet moving on a linear chain. The spreading is not yet visible. The chain is actually disordered weakly, but the effects of disorder are not obvious for the short time interval shown.

IV. MODES OF TIME EVOLUTION

The aim of this article is to discover the nature of the normal modes of a disordered lattice. The wave-packet construction just reviewed plays a crucial role. It is the method by which we understand the nature of the normal modes of the perfect ordered chain. Specifically, they are traveling waves, spatially extended with equal amplitude on all lattice points, but also they build pulse-like disturbances which propagate *ballistically*. That is, they have a velocity v_0 of propagation. A similar wave-packet construction for the disordered lattice will reveal much about the nature of the normal modes.

Table I gives the various characteristic forms of time evolution of a pulse that may be expected. Two separate effects can happen because of disorder. One is scattering of waves from the disorder. The other is localization. Scattering causes the phase of the normal mode to become disorganized after a distance known as the “mean free path,” denoted by l_μ . For distances longer than l_μ a disturbance can no longer propagate ballistically but can still propagate diffusively. In one dimension, the diffusion equation shows that a disturbance localized in a spatial region of width b at $t=0$ spreads over a root-mean-square distance $\sqrt{(b^2 + 2Dt)}$, where D is the diffusion constant. Localization means that diffusive propagation is prohibited at length scales longer than the localization length ξ_μ . On a one-dimensional lattice with weak disorder, there is a wide range of frequencies for which $l_\mu \ll \xi_\mu$, allowing diffusive propagation to occur over significant times and distances before ultimately reaching a maximum distance of ξ_μ and stopping.

V. NORMAL MODES OF THE DISORDERED CHAIN

What is the nature of the normal modes when the chain is disordered? For a finite chain of N “atoms,” the normal modes can be explicitly found on a computer by finding the eigenvalues ω_μ^2 and eigenvectors $|\mu\rangle$ of an $N \times N$ real symmetric matrix, as explained in Appendix B. The index μ runs from 0 to N and labels the normal modes. The notation $|\mu\rangle$ denotes a column vector whose elements $\langle 1|\mu\rangle = u_{1\mu}, \dots, \langle n|\mu\rangle = u_{n\mu}, \dots$ contain the displacement pattern of the μ th normal mode at the n th atom. A solution of Newton’s laws $u_1(t), \dots, u_n(t), \dots$ is compactly denoted by the column vec-

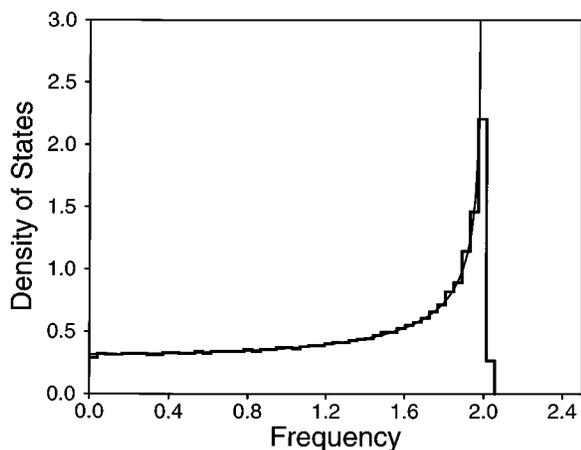


Fig. 3. Calculated vibrational density of states for the disordered chain compared with the exact density of states of the ordered chain [Eq. (A6)]. As shown here and in Fig. 4, frequency is measured in units of $\Omega = \sqrt{k/M}$. The perfect chain has $\omega_{\max}=2$ in these units. In the rest of the paper, time is measured in units of the period $2\pi/\omega_{\max}$ of the fastest vibration, and the value of ω_{\max} is 2π .

tor $|U(t)\rangle$. The symbol $|n\rangle$ denotes a column vector which is all zeros except for a 1 in the n th entry, so that $\langle n|U(t)\rangle$ denotes $u_n(t)$. The normal modes span the space of possible states $|U\rangle$ of the chain, and can be chosen to be orthonormal $\langle \mu|\mu'\rangle = \delta_{\mu,\mu'}$. An example of normal modes and vector notation for a four-atom chain is given in Appendix B.

Figure 3 shows a histogram of the density of vibrational states of a 3000 “atom” chain. The spring constants k_n were chosen in the form $k_n = k(1+r_n)$, where r_n is chosen by a random number generator and is uniformly distributed in the interval $(-0.07, 0.07)$. This corresponds to a weak disorder. The corresponding answers for a strongly disordered case with r_n randomly distributed in $(-0.7, 0.7)$ can be seen in a recent paper.¹¹ The result is compared with Eq. (A6) for the perfect chain. The small random disorder hardly affects the overall frequency spectrum, except to broaden the peak at $\omega = \omega_{\max}$.

A very useful diagnostic for localization is the “participation ratio” p_μ of the normal mode $|\mu\rangle$ introduced by Bell and Dean.¹² The inverse of this is defined by

$$1 = \langle \mu|\mu\rangle = \sum_n |\langle n|\mu\rangle|^2, \quad (10)$$

$$1/p_\mu = \sum_n |\langle n|\mu\rangle|^4. \quad (11)$$

Equation (10) just states a normalization condition on the normal modes. For a traveling wave in a perfect crystal, the amplitude is the same at every site, so $|\langle n|\mu\rangle|^2 = 1/N$, and $1/p_\mu = 1/N$. For a hypothetical state which is localized on a single point, $|\langle n|\mu\rangle|^2$ is zero everywhere except at that point where it is 1, and $1/p_\mu = 1$. Thus the participation ratio p_μ measures the number of sites where the state $|\mu\rangle$ has a significant amplitude. For a one-dimensional system, the localization length ξ_μ is $p_\mu a$. Figure 4 shows the results for the disordered chain, averaged over modes with ω_μ in frequency bins.

It is important to realize that the actual object of interest is not the 3000 “atom” chain (corresponding to 1 μm length in

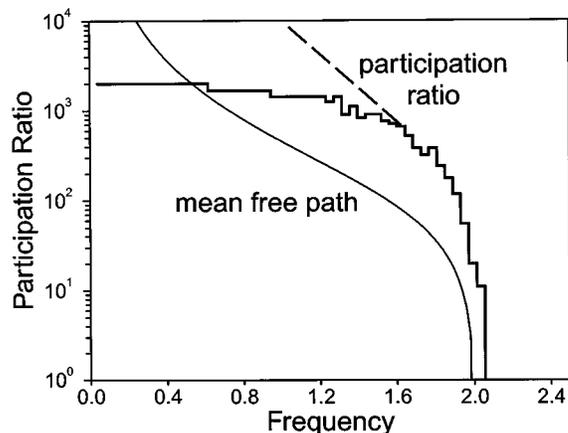


Fig. 4. The participation ratio $p = \xi/a$ of the vibrational normal modes of the disordered chain, calculated according to Eq. (11), is shown as a histogram, averaged over frequency bins. The dashed line is a schematic extrapolation to larger size chains. The mean free path l/a calculated from Eq. (12) is shown as the smooth curve.

actual atomic dimensions) but instead a “macroscopic” system of much longer length. We would like to extract from our calculation information which applies to systems of unlimited length. Suppose we had a much larger computer and could manage 3×10^6 “atoms” (or 1-mm sample.) The spectrum shown in Fig. 3 would be unchanged. However, the modes in Fig. 4 which have localization length $1000a < \xi = pa < 3000a$ would in the next calculation have longer localization lengths. The fact that ξ saturates at $\approx 2000a$ in Fig. 4 is (from this point of view) an artifact of the finite size of the sample studied. It is known¹³ that the true behavior of ξ as a function of eigenfrequency ω is $\xi \propto \omega^{-2}$. For any finite size chain, the normal modes at low enough ω will extend from one end of the chain to the other, but for a larger chain, the modes at the same frequency will be localized. For an infinite chain, only modes of infinitely small frequency are delocalized. As the length N of a chain increases, the number of modes which extend throughout the chain should increase as $N^{1/2}$, but the fraction of modes which appear delocalized should decrease as $N^{-1/2}$.

The other important property of the normal modes of the disordered chain is their mean free path l_μ . There is no formula which enables l_μ to be calculated from just the eigenvector $|\mu\rangle$. The definition begins by asserting that to first approximation we have traveling wave states with wave vector Q . Then the mean free path l_Q is defined as the distance a wave packet (of central wave vector Q) can travel on average before its trajectory is randomized by scattering from the disorder. In the next section a computer experiment will implement this definition. Disorder is put in by choosing a specific set of spring constants $k_n = k(1+r_n)$ with r_n randomly and uniformly distributed in the interval $(-R, R)$, where R serves as the small parameter of the theory. A theoretical value for l_Q can be found by perturbation theory. The answer, derived in Appendix A, is

$$\frac{l_Q}{a} = \frac{3}{4} \left(\frac{1}{R} \right)^2 \left(\frac{\omega_{\max}^2 - \omega_Q^2}{\omega_Q^2} \right). \quad (12)$$

This result is shown in Fig. 4. Note that l_Q diverges as $1/R^2$ as the strength of the perturbation R goes to zero, and also

(similar to ξ) as $1/\omega_Q^2$ as the frequency ω_Q goes to zero. When the same calculation is done for three-dimensional vibrational waves, the long-wavelength mean free path diverges as $1/\omega_Q^4$, which is the vibrational version of Rayleigh scattering.

VI. TIME EVOLUTION ON THE DISORDERED CHAIN

Using Fig. 4, we have chosen an appropriate frequency $\omega_0 = 1.581\Omega = 0.79\omega_{\max}$ and wave vector $Q_0 = 1.8235/a$ for computer experiments with a wave packet. These choices correspond to a predicted mean free path of $92a$ and localization length of $740a$. Then there is a sequence of length scales λ (wavelength) $\ll l$ (mean free path) $\ll \xi$ (localization length) $\ll L$ (sample size). Actually the sample size is only four times larger than the localization length. A wave localized with $\xi \approx L/4$ has exponential tails on both sides, which causes the disturbance to interact with the boundary. To avoid such surface effects, we have embedded the 3000 atom section in the middle of a 15 000 atom chain.

What is the appropriate definition of a wave packet on a disordered chain? Our answer is to use the perfect chain formulas, Eqs. (6)–(8), to pick displacements and velocities at time $t=0$. This gives a candidate initial pulse. For a perfect chain, by construction, this pulse is built from eigenstates whose frequencies are confined to the window $\omega_0 \pm v_0/b$. For the disordered chain, the exact eigenmodes differ from the plane-wave states of the perfect chain, so there is no longer perfect confinement of the frequency spectrum of the pulse to this window. Our aim is to discover the nature of normal modes of the disordered chain for frequencies near ω_0 . Therefore we “filtered” the initial pulse by expanding in the exact eigenstates $|\mu\rangle$ and then multiplying each amplitude by the factor $\exp[-(\omega_\mu - \omega_0)^2/2\delta\omega^2]$.¹⁴

The pulse can now be propagated forward in time, using either Eq. (C5) or else direct forward integration in time of Newton’s laws, as explained in Appendix D. The two procedures gave the same result.

The energy on the chain is distributed in time-varying fashion between kinetic energy of moving atoms and potential energy of distorted chains. There are several sensible ways, and no unique way, of defining a quantity $E_n(t)$, the local energy at time t associated with atom n . For example, one can use all the kinetic energy of atom n and half the potential energy of each of the two connected springs. A sensible definition should be additive, $\sum_n E_n(t) = E_{\text{tot}}$. It should make no substantive difference which sensible definition is used. Our definition, Eq. (C6), explained in Appendix C, is novel and is chosen because of mathematical and computational elegance, but it is not necessary to use such an abstract definition. Once the local energy $E_n(t)$ is defined, one can use it graphically and also algebraically to define the center $R(t)$ of a pulse and the width $\sqrt{\langle r^2(t) \rangle}$ of a pulse:

$$R(t) \equiv \frac{\sum_n n a E_n(t)}{\sum_n E_n(t)}, \quad (13)$$

$$\langle r^2(t) \rangle \equiv \frac{\sum_n (na - R(t))^2 E_n(t)}{\sum_n E_n(t)}.$$

Figure 5 shows the spatial evolution of the energy (defined in Appendix C) of the wave for the first ten units of time.

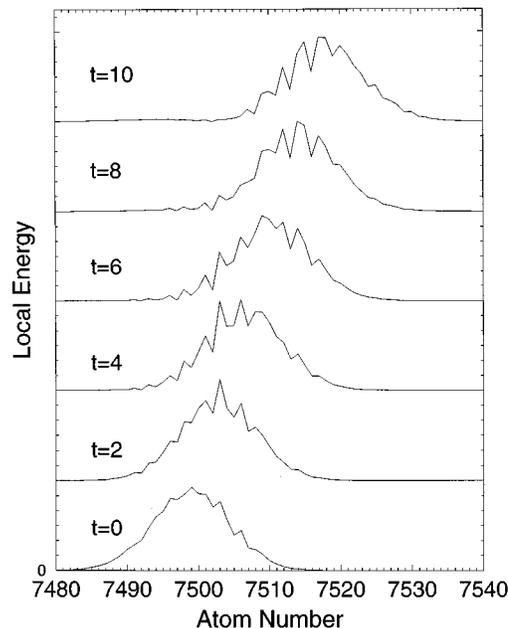


Fig. 5. The local energy at fairly short times.

The detailed local energy distribution evolves in a complicated way, but on this time scale, no broadening or other significant change of shape of the envelope of the pulse can be seen with resolution of a few percent. Within the envelope an interesting substructure is starting to develop, which is mentioned again at the end of Sec. VI. If the chain had been perfect, the pulse broadening predicted by Eq. (9) would have been $\approx 1\%$ at $t=10$, consistent with the figure. The measured full width at half-maximum of the energy distribution is $\approx 12a$, which agrees with the formula $2\sqrt{\ln 2}b$ for the Gaussian profile of Eq. (9).

At somewhat longer times, shown in Fig. 6, several new effects are seen. By $t=50$ the main part of the pulse has traveled ballistically a distance of $93a$, 3% less than predicted from the group velocity $v_0 = 1.92$ for the perfect lattice. The width of this main pulse is 60% wider than at $t=0$, exactly as predicted by Eq. (9) for the perfect lattice. However, the pulse height has shrunk by a factor of 2; the area under the leading pulse is not conserved. Inspection of the upper curve of Fig. 6, or equivalently, the lower curve of Fig. 7, shows that the missing energy is mostly in a few secondary pulses which have split off the main pulse at intermediate times and are propagating backward. Apparently, at approximately $t=7$ and $t=19$ the pulse encountered some particularly severe fluctuations in the spring-constant disorder which reflected part of the incident energy. By $t=200$, shown in the top panel of Fig. 7, most of the energy is in secondary pulses with directions of propagation which are effectively random. The wave is now well out of the ballistic and into the diffusive regime.

Although the ballistic leading edge of the pulse continues to contain quite a lot of the energy until at least $t=200$, the center of energy, defined in Eq. (13), already begins to deviate from a ballistic trajectory as early as $t=50$. Figure 8 shows the time evolution of the center of energy for two pulses, prepared with identical recipes but started at two different locations that are 25 “atoms” apart. By $t=200$ the center reaches its maximum excursion of 150, and then pro-

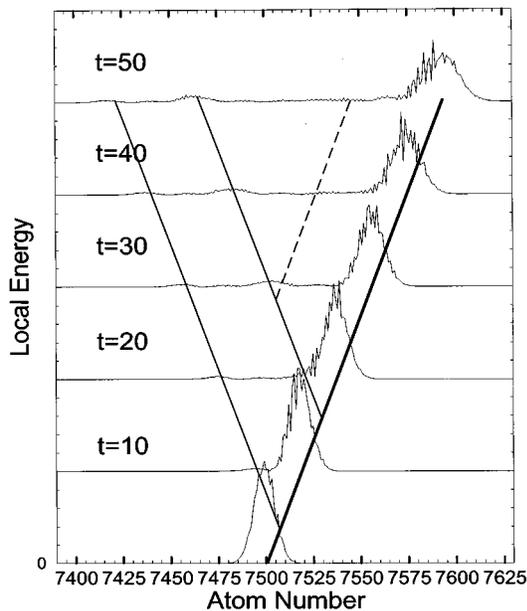


Fig. 6. The local energy at medium times. The bold line represents the path of the center of energy of the leading pulse. There are also secondary pulses traveling from right to left at larger times, whose paths are represented by thinner solid lines, and one of the many weak multiply scattered pulses is indicated by the dashed line. The top panel is repeated on a different scale in Fig. 7.

ceeds to wander slowly by ± 25 “atoms.” This wandering seems chaotic, but in fact, in the technical sense of “chaos” it is just the opposite. Chaotic behavior is by definition a divergence of initially close trajectories which grows exponentially in time. It is quite remarkable how “nonchaotic” Fig. 8 is. Absence of chaos is a fundamental property of all systems of coupled harmonic oscillators, but we did not anticipate either the long-time fluctuations of Fig. 8 or the insensitivity to starting point.

Quantum mechanics enriches classical mechanics by offering a vivid particle interpretation of wave behavior. The pulse evolution shown in Figs. 5–7 is equivalent to the evolution of $|\psi|^2$ for a quantum electron on a chain of atoms. It is a “band” electron experiencing weak scattering from disorder in the lattice. For a while it propagates ballistically, corresponding to a single classical trajectory, but then it scatters and no longer has a single deterministic route. Instead, it is a superposition of trajectories. The waveform gives a statistical description of where the particle has gone. For some purposes it is adequate to ignore interference between different trajectories, and to think of the time evolution as an ensemble of random walks. At this level, a Boltzmann gas theory description works, and describes the time evolution of this ensemble in terms of scattering probabilities at different sites. This is the spirit behind the mean free path calculation of Appendix A.

As discussed in Sec. V, the mean free path l is predicted to be $92a$, and the localization length ξ is found to be $740a$. This enables us to understand Fig. 8. After ballistically propagating a distance of about l , the propagation becomes randomized and no further change of the center of energy is expected, except for some statistical fluctuations which depend on the initial conditions. Our two pulses have similar initial conditions and propagate through the same disordered regions. Localization should not be an important factor until

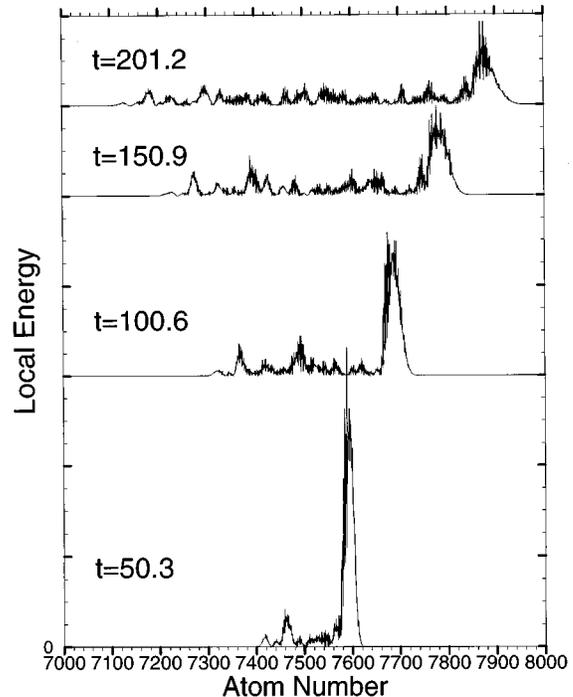


Fig. 7. The local energy at fairly long times.

the wave has propagated a distance ξ . Ballistic propagation at a velocity of 1.92 would reach a distance ξ in $t \approx 400$. However, by this time there is little remaining ballistic behavior, and theory predicts diffusive spreading with $\langle r^2 \rangle = 2Dt$. Statistical theory gives in one dimension $D = vl$, which is predicted to be 180 for our pulse. Diffusion should then be observed for times until $2Dt = \xi^2$, or $t \approx 1500$.

The squared width of the energy pulse is defined in Eq. (13), and plotted in Fig. 9. For times up to $t \approx 1000$ the numerical data agree well with the diffusive prediction, except that the value of D obtained from the linear slope is ≈ 300 rather than 180. If this revised value of D is used to predict when the localization length is reached, the answer, $t \approx 900$, agrees very well with the breakdown of linear behavior of $\langle r^2 \rangle$ vs t seen in Fig. 9.

For times $t > 1000$, a new regime occurs, as is shown in Fig. 10. The pulse no longer varies much in time, at least

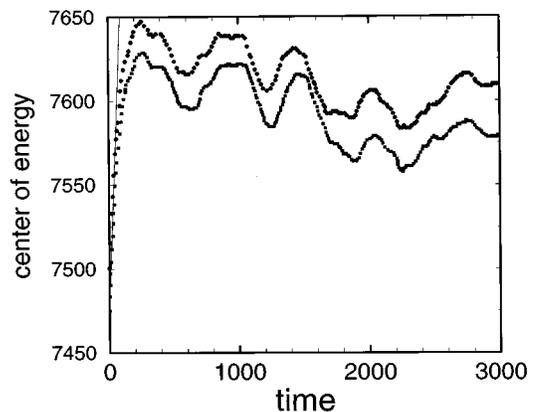


Fig. 8. The center of energy vs time. The straight line drawn near the vertical axis represents ballistic propagation with group velocity 1.92.

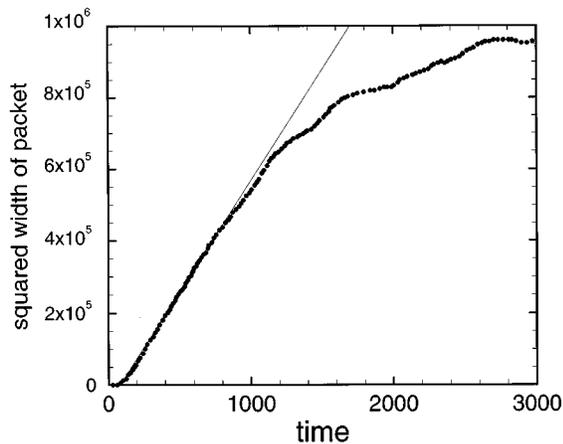


Fig. 9. Squared width of the packet vs time. The straight line represents diffusive propagation with $\langle r^2 \rangle = 2Dt$ and $D = 309$.

until details are examined. Energy was initially inserted into normal modes of frequency ω_μ near ω_0 , but arranged to interfere destructively, except in a narrow spatial region of width b near R_0 . For $t > 1000$, the original pattern of destructive interference has disappeared, and the full spatial extent of the eigenstates is seen in the pulse. Since the eigenstates decay exponentially for distances greater than $\xi \approx 740$, the pulse cannot go farther and is localized. As time evolves, the relative phases of the different localized normal modes changes, and the detailed spatial pattern of the energy pulse changes. This leads to a surprising secular fluctuation of the center of energy seen in Fig. 8 and a weak fluctuation in the width seen in Fig. 9.

A careful look at Figs. 6, 7, and 10 shows an effect which contradicts a too-classical particle interpretation. The local

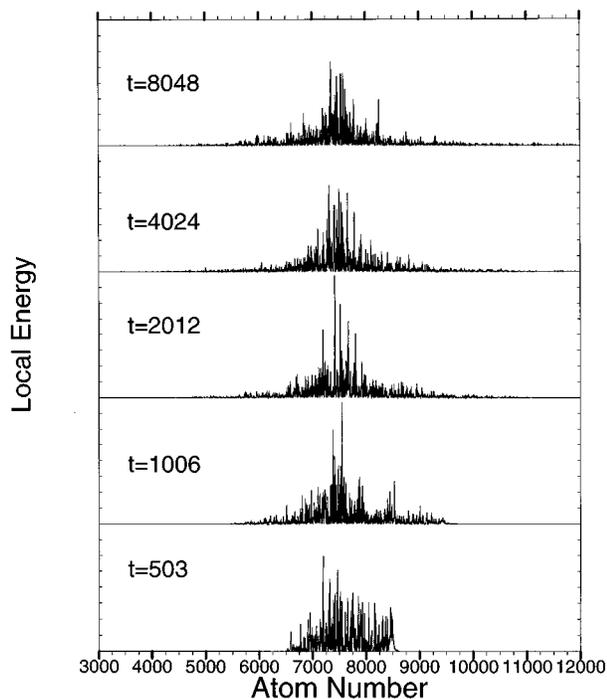


Fig. 10. The local energy at very long times.

energy does not spread uniformly in space, but is very spiky. This is not an artifact, but an interesting interference effect which is not contained in the description in terms of diffusion. Scattered waves from different spatial fluctuations of spring constants interfere strongly with each other, so that parts of the chain have large oscillation amplitudes and other parts have nearly zero amplitude, in a pattern which evolves in time. This effect is noticeable long before localization sets in. However, it is (in a sense) a precursor of localization, because the origin of localization has been traced to destructive interference between incident and backscattered wave components. The appearance of this interference effect before the onset of localization is one of a class of effects known in the solid state literature as “weak localization.”^{15,16}

VII. HIGHER DIMENSIONS

Vibrations in solids are generally three dimensional in character. Unfortunately, computer simulations in three dimensions become much harder. A matrix size of 3000×3000 no longer handles a spatial length of $3000a$, but (remembering the three spatial degrees of freedom for each atom) only $10a$, which is short enough that localization effects become mixed with finite size effects. The most important new effect in $d = 3$ is a sharp boundary in the frequency spectrum which separates states which are strictly delocalized (impossible in lower dimensions) from states which are localized. Near the boundary, the localized states have very long values of ξ , diverging as the boundary is approached. Farther away from the boundary, the localization lengths can become very short, if the disorder is great enough. On the delocalized side of the boundary, the extended states have very short mean free paths, going close to zero as the boundary is approached. Therefore, ballistic propagation does not occur in this part of the spectrum, and states can be called “intrinsically diffusive.” Wave-packet-like states formed in this region of the spectrum show neither a ballistic nor a localized regime, and continue diffusing until they fill the sample. On the localized side of the boundary, but close enough that ξ_μ is large, one could perhaps construct superpositions of normal modes, like wave packets, which would be initially localized on a shorter length scale than ξ_μ . The time evolution of such a disturbance would be diffusive, with no ballistic region, until the size of the disturbance equaled ξ_μ , at which time further spreading would stop. It is probably impossible in three dimensions to find a spectral region where ballistic propagation as well as diffusion and localization can all be seen as a wave packet evolves. Verifying these ideas numerically is not easy, and controversy still remains.

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APPENDIX A: PERTURBATIVE TREATMENT OF WEAK DISORDER

Localization cannot be found by adding disorder perturbatively to the theory of a perfect crystal. The fact that modes

are always localized in one dimension indicates that ordinary perturbation theory cannot succeed at long times. However, for a wave packet on a weakly disordered chain, there is an interval of time between the scattering time $\tau=l/v$ and the time when the distance $\sqrt{(2Dt)}$ of diffusion equals the localization length ξ , during which the effect of localization is unimportant and perturbation theory gives a useful description of diffusion.

Even though the pulse propagation problem is purely classical, the quantum version offers a simpler treatment. As historical evidence for this, heat conduction in insulators was first understood qualitatively by Debye in 1912 using classical ideas, but only after Peierls introduced the quantum version in 1929 did the theory become complete and predictive. The high T limit of Peierls's theory gives the correct classical theory which Debye's work foreshadowed. The derivation of Eq. (12) is a technical detail which the reader is free to skip.

First write the Hamiltonian in terms of quantum raising and lowering operators a_Q^\dagger and a_Q for the uncoupled oscillators Q of the ordered chain,

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1, \quad (\text{A1})$$

$$\mathcal{H}_0 = \sum_Q \hbar \omega_Q \left(a_Q^\dagger a_Q + \frac{1}{2} \right), \quad (\text{A2})$$

$$\mathcal{H}_1 = \frac{1}{N} \sum_{Q,Q'} V_{QQ'} a_Q^\dagger a_{Q'}. \quad (\text{A3})$$

\mathcal{H}_0 is the ordered chain, and \mathcal{H}_1 contains the random disorder. The frequency ω_Q is, as before, $\omega_{\max} |\sin(Qa/2)|$, where the maximum frequency is $\omega_{\max} = 2\sqrt{K} = 2\Omega$. The scattering potential $V_{QQ'}$ depends on the particular choice of random numbers K_n . We are interested in the average rate of scattering, and can average this over an ensemble of randomly prepared chains. The standard perturbative formula is

$$\frac{1}{\tau_Q} = \frac{2\pi}{N\hbar} \sum_{Q'} \langle |V_{QQ'}|^2 \rangle \delta(\hbar\omega_Q - \hbar\omega_{Q'}), \quad (\text{A4})$$

where the angular brackets denote the ensemble average. It is not hard to show that

$$\langle |V_{QQ'}|^2 \rangle = \frac{1}{6} (\hbar\omega_Q)(\hbar\omega_{Q'}) R^2. \quad (\text{A5})$$

The only significant Q' dependence remaining in the sum of Eq. (A4) is a factor of the vibrational density of states $\mathcal{A}(\omega_Q)$, namely,¹⁷

$$\mathcal{A}(\omega) = \frac{1}{N} \sum_Q \delta(\hbar\omega_Q - \hbar\omega) = \frac{2}{\pi\hbar} \frac{1}{\sqrt{\omega_{\max}^2 - \omega^2}}. \quad (\text{A6})$$

This is the formula which is plotted in Fig. 3. Finally, Eq. (12) for the mean free path $l_Q = v_Q \tau_Q$ follows by combining Eqs. (A4) and (A5) and using the formula $v_Q = (a/2) \sqrt{\omega_{\max}^2 - \omega_Q^2}$.

APPENDIX B: VECTOR NOTATION

Displacement information for a chain of N masses can be encoded in a vector $|U(t)\rangle$ which has N components, one for each "atom" $u_n(t) = \langle n|U(t)\rangle$. As a specific illustration, consider a line of four masses connected by springs k_n . It is

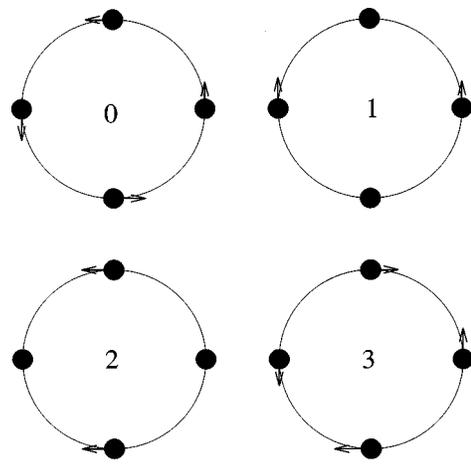


Fig. 11. A chain of four point masses, with periodic boundary conditions. For equal spring constants, the patterns of the four vibrational normal modes are shown. The mass points are numbered 1,2,3,4 in the counterclockwise direction starting with the rightmost point.

convenient to use periodic or Born-Von Karman boundary conditions, which can be visualized in several ways. One visualization is to embed the four atoms in an infinite line of atoms, enforcing the condition $u_n(t) = u_{n+4}(t)$ which says that each group of four atoms has an identical motion. Another visualization is to bend the line into a ring as in Fig. 11. Let K_n denote k_n/M . In vector form, Newton's equations of motion are

$$\frac{d^2|U\rangle}{dt^2} = -\mathbf{K} \cdot |U\rangle, \quad (\text{B1})$$

where \mathbf{K} is $1/M$ times the 4×4 matrix of second derivatives of the potential,

$$\mathbf{K} = \begin{pmatrix} K_4 + K_1 & -K_1 & 0 & -K_4 \\ -K_1 & K_1 + K_2 & -K_2 & 0 \\ 0 & -K_2 & K_2 + K_3 & -K_3 \\ -K_4 & 0 & -K_3 & K_3 + K_4 \end{pmatrix}, \quad (\text{B2})$$

$$|U\rangle = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}.$$

The real-symmetric matrix \mathbf{K} has some special properties which continue to hold for chains of atoms of arbitrary length N , namely: (1) on the diagonal occur the positive numbers $K_{n-1} + K_n$; (2) on the adjacent subdiagonals occur the negative numbers $-K_n$; (3) all further subdiagonals are filled with zeros except for the far corners which contain $-K_N$; (4) the sum of the elements in each row and in each column is zero. This last property expresses the translational invariance of the potential energy, namely, the fact that if each atom (at position $na + u_n$) is given an additional constant displacement δ , the potential energy is unchanged and there is no additional restoring force. It is also easy to prove that for any displacement vector $|U\rangle$, the quantity $\langle U|\mathbf{K}|U\rangle$ is just $2V/M$, which is twice the potential energy per unit mass stored in that displacement pattern, a non-negative number. Therefore the matrix \mathbf{K} is a non-negative matrix.

The eigenvalues and eigenvectors of K play a special role. Denote these vectors by $|\mu\rangle$ and the corresponding eigenvalues by ω_μ^2 . The eigenvalues of a non-negative real-symmetric matrix are real and non-negative, so they have real and non-negative square roots ω_μ , which are the frequencies of the “normal modes” of oscillation. The motion given by $A_\mu|\mu\rangle\cos(\omega_\mu t + \phi_\mu)$ (with A_μ and ϕ_μ arbitrary real numbers) is a solution of Newton’s laws. This solution has a stationary displacement pattern which oscillates in time sinusoidally. It is a standing wave “stationary state” or normal mode. For the chain of four atoms shown in Fig. 11, the displacement patterns of the four normal modes are easy to find if the springs $k_n = M\Omega^2$ have all equal values. The normal mode displacements are indicated in the figure, and are given by the orthonormal vectors

$$\begin{aligned} |0\rangle &= \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, & |1\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix}, \\ |2\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix}, & |3\rangle &= \frac{1}{2} \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}. \end{aligned} \quad (\text{B3})$$

The corresponding eigenfrequencies are $\omega_0=0$, $\omega_1=\omega_2=\sqrt{2}\Omega$, and $\omega_3=2\Omega$. Notice that the mode labeled $|0\rangle$ has every atom displaced equally, which means that it is a uniform translation. Therefore this mode has no restoring force; the corresponding frequency is 0. Rather than a sinusoidal oscillation, the motion corresponding to this vector is $|0\rangle(u_0+v_0t)$, i.e., a translation with constant velocity. Modes $|1\rangle$ and $|2\rangle$ are degenerate; therefore linear combinations of $|1\rangle$ and $|2\rangle$ are also normal modes. In particular, the modes $(|1\rangle \pm i|2\rangle)/\sqrt{2}$ are traveling waves, whereas the representation in Eq. (B3) using real numbers corresponds to standing waves.

The most general solution of Newton’s laws is a superposition of normal mode oscillations with arbitrary amplitudes and phases. As an example, the initial value problem can be solved once the initial positions $|U(0)\rangle$ and initial velocities $|V(0)\rangle$ are known. It is easy to verify (from the completeness and orthogonality of the eigenvectors $|\mu\rangle$) that the solution is

$$\begin{aligned} |U(t)\rangle &= \sum_\mu \left[|\mu\rangle\langle\mu|U(0)\rangle\cos(\omega_\mu t) \right. \\ &\quad \left. + |\mu\rangle\langle\mu|V(0)\rangle\frac{\sin(\omega_\mu t)}{\omega_\mu} \right], \end{aligned} \quad (\text{B4})$$

$$\begin{aligned} |V(t)\rangle &= \sum_\mu [|\mu\rangle\langle\mu|V(0)\rangle\cos(\omega_\mu t) \\ &\quad - |\mu\rangle\langle\mu|U(0)\rangle\omega_\mu \sin(\omega_\mu t)]. \end{aligned} \quad (\text{B5})$$

For the case $|\mu\rangle=|0\rangle$, we use the limit as ω_μ approaches zero, $\sin(\omega_\mu t)/\omega_\mu \rightarrow t$.

APPENDIX C: COMPLEX NOTATION; RELATION TO SCHRÖDINGER EQUATION

For a single harmonic oscillator, the solution of the initial value problem, $x(t)=x(0)\cos(\omega t)+[v(0)/\omega]\sin(\omega t)$ is often

written as $x(t)=\text{Re}[A\exp(-i\omega t)]$, where A is a complex number of modulus $|A|=\sqrt{x(0)^2+v(0)^2/\omega^2}$ and phase $\phi=\tan^{-1}(v(0)/\omega x(0))$. There is more than one way to generalize this notation to the problem of coupled oscillators, but the following version seems particularly interesting. Define a complex vector

$$|W(t)\rangle=|V(t)\rangle-i\Omega|U(t)\rangle. \quad (\text{C1})$$

The real vectors $|V(t)\rangle$ and $|U(t)\rangle$ are defined as in Eqs. (B5) and (B4). The matrix Ω obeys $\Omega^2=K$; that is, it is the positive square root of the matrix K . To be explicit, Ω can be written as

$$\Omega=\sum_\mu \omega_\mu|\mu\rangle\langle\mu|. \quad (\text{C2})$$

To be even more explicit, for the four-atom chain of the previous section, when K_i is a constant, K , the matrix Ω can be constructed using Eqs. (C2) and (B3), and is

$$\Omega=\frac{K}{2} \begin{pmatrix} 1+\sqrt{2} & -1 & 1-\sqrt{2} & -1 \\ -1 & 1+\sqrt{2} & -1 & 1-\sqrt{2} \\ 1-\sqrt{2} & -1 & 1+\sqrt{2} & -1 \\ -1 & 1-\sqrt{2} & -1 & 1+\sqrt{2} \end{pmatrix}. \quad (\text{C3})$$

The square of this matrix is indeed Eq. (B2).

The complex vector $|W(t)\rangle$ encodes almost all dynamical information about the system of oscillators. Velocities are in the real part of $|W(t)\rangle$ and positions (except for the absolute position of the center of mass) are in the imaginary part. Center of mass position information is lost because Ω operating on a constant vector $|U\rangle$ gives zero. In technical language, $|W(t)\rangle$ is orthogonal to the null space of Ω and K , while the null space contains the center of mass information. The center of mass moves with uniform velocity, and we choose a reference frame at rest with respect to the center of mass.

One of the interesting things about the vector $|W(t)\rangle$ is that Newton’s laws become

$$i\frac{d|W(t)\rangle}{dt}=\Omega|W(t)\rangle. \quad (\text{C4})$$

If Ω is reinterpreted as a Hamiltonian, and $|W(t)\rangle$ as a state vector, then this is a time-dependent Schrödinger equation. The solution is

$$|W(t)\rangle=e^{-i\Omega t}|W(0)\rangle, \quad (\text{C5})$$

which is just a symbolic version of Eqs. (B4) and (B5). The classical one-dimensional lattice vibration problem is isomorphic to the quantum problem of a single electron propagating on a chain of atoms, each of which has a single orbital available for the electron. The basis vector $|n\rangle$ refers in the quantum problem to the orbital on site n , and $\langle n|\Psi(t)\rangle$ (analogous to $\langle n|W(t)\rangle$) is the amplitude for the electron to be on this site. The Hamiltonian matrix H has elements H_{mn} to hop from site m to site n which are the quantum analog of Ω_{mn} , the matrix elements of the square root of the spring-constant matrix.

There is one point of difference between the classical wave on the chain and the quantum electron, namely, vector $|Q=0\rangle$, which has equal amplitude at every site, is a uniform translation of the classical lattice, with no restoring force, and thus a corresponding null eigenvalue. This has no

analog in the electron propagation problem. The uniform translation of the lattice guarantees the existence of soundlike propagation. That is, for a long chain there must be eigenstates of the vibrational problem which look locally like uniform translations and have very low frequencies. Such states are uniquely resistant to localization, with diverging localization lengths as the frequency goes to zero.

The usefulness of the Schrödinger form of Newton's laws in our case is the following. The Schrödinger equation has a conserved quantity, $\langle \Psi(t) | \Psi(t) \rangle$, or the norm of the wave function, which expresses particle number conservation. The corresponding lattice quantity, $\langle W(t) | W(t) \rangle$, must also be conserved, and it is easy to see that it is just $2E/M$, twice the total (kinetic plus potential) energy per unit mass of the oscillating masses. The importance of this is that since $\langle W(t) | W(t) \rangle = \sum_n |\langle n | W(t) \rangle|^2$, we have just written the energy as an additive sum of single-site quantities, and we are entitled (if we wish) to define

$$E_n(t) \equiv (M/2) |\langle n | W(t) \rangle|^2 \quad (\text{C6})$$

as the local energy $E_n(t)$ at site n . In the quantum problem, we are curious about the time evolution of $|\langle n | \Psi(t) \rangle|^2$, the occupancy of site n ; similarly, in the classical problem we will study the time evolution of $E_n(t)$, a quantity which appears naturally in the equations of motion once we adopt this notation.

APPENDIX D: NUMERICAL METHODS

A workstation with 256 Mbytes of memory can handle matrices of size 3000×3000 . Like the example of Appendix B, we chose periodic boundary conditions at the ends of the 3000 "atom" chain. The resulting 3000 eigenvectors, each containing 3000 entries, using double precision (8-byte words) occupies 72 Mbytes of storage—roughly the same as a 12-volume encyclopedia. The matrix diagonalization takes a few hours on an IBM series 6000 computer. In principle, since the matrix for a chain is banded, faster methods can be used, but for our purposes it was not necessary.

Once the eigenvectors and eigenvalues are known, and the initial values of the displacement and velocity of the pulse are given, the future values $|W(t)\rangle$ can be found from the initial value using Eq. (C5). In practice this means a sequence of vector product calculations,

$$\langle n | W(t) \rangle = \sum_{\mu} \langle n | \mu \rangle e^{-i\omega_{\mu}t} \langle \mu | W(0) \rangle, \quad (\text{D1})$$

which takes N^2 operations to update the N complex numbers $\langle n | W(t) \rangle$. For roughly the same computational time, and much less storage, one can calculate a series of N updates $\langle n | W(t_i) \rangle$ for $t_i = (t_1, t_2, \dots, t_N)$ equally spaced time intervals by direct forward integration of Newton's laws with a suitably small $\Delta t = t_2 - t_1$. The algorithm we used is a simple difference method,¹⁸ sometimes called the "Verlet algorithm,"¹⁹

$$u_n(t + \Delta t) = 2u_n(t) - u_n(t - \Delta t) + \frac{1}{m} F_n(t) \Delta t^2, \quad (\text{D2})$$

which can be derived from the expansion $u_n(t \pm \Delta t) = u_n(t) \pm \dot{u}_n(t) \Delta t + (1/2m) F_n(t) \Delta t^2$ by adding the plus and minus equations. This algorithm is correct up to order Δt^4 and gives very accurate answers for oscillator problems when Δt is chosen $\approx 1\%$ of the period of the fastest oscillator. Thus

we can get a complete trajectory over 30 units of time with the same expense as a single update using Eq. (D1) once for an arbitrary time. We have verified that the two methods agree well up to times of 700 or greater. Knowledge of eigenvectors was necessary to set up the wave packet; this knowledge was used to find $|W(-\Delta t)\rangle$, which is needed to start Eq. (D2).

Once the leading edges of the propagating wave packet reach the ends of the 3000 "atom" chain, the vector method Eq. (D1) begins to yield spurious effects from the wrapping around of the chain implicit in periodic boundary conditions. Hard wall or free boundary conditions would yield equally spurious reflection effects. These are all avoided by embedding the 3000 "atom" chain in a much longer chain whose spring constants are chosen by the same random recipe, and using forward integration of Newton's law, Eq. (D2), for the long chain.

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