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Schrödinger Correspondence Applied to Crystals

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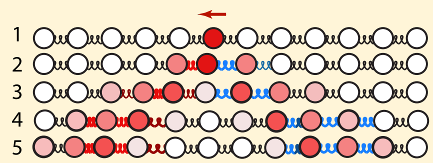
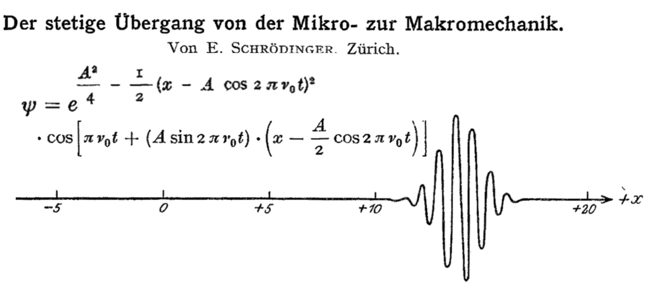
ABSTRACT: In 1926, E. Schrödinger showed that the mean position and mean momentum of the displaced ground state in a harmonic oscillator obey the equations of motion of the classical oscillator. This Schrödinger Correspondence Principle, extended to an N-dimensional harmonic oscillator, is an intuitive and powerful way to approach many aspects of harmonic solids by converting the quantum-mechanical problems to the classical ones. For the application of the correspondence principle, the concepts of the phonon and its pseudomomentum are clarified, and the importance of taking into account the center-of-mass momentum is explained. Also, the concept of the antiphonon is introduced through the examples of physical processes in a line and a ring of atoms. With the correspondence principle, the quantum behavior of harmonic solids under a Mössbauer-like kick is analyzed classically, and the simulation verified the formation of an antiphonon.



1. INTRODUCTION

In 1926, Schrödinger made the connection between the dynamics of a displaced quantum ground-state Gaussian wave packet in a harmonic oscillator and classical motion in the same harmonic oscillator[1] (see Figure 1). The mean position



Der stetige Übergang von der Mikro- zur Makromechanik.

Von E. Schrödinger. Zürich.

$$\psi = e^{\frac{A^2}{4} - \frac{1}{2}(x - A\cos 2\pi\nu_0 t)^2} \cdot \cos\left[\pi\nu_0 t + (A\sin 2\pi\nu_0 t)\cdot\left(x - \frac{A}{2}\cos 2\pi\nu_0 t\right)\right]$$

Figure 1. Photocopy from Schrödinger's 1926 paper. Reprinted with permission from ref 1. Copyright 1926 Springer-Verlag.

of the Gaussian (its guiding position center) and the mean momentum (its guiding momentum center) follow classical harmonic oscillator equations of motion, whereas the width of the Gaussian remains stationary if it initially was a displaced (in position, momentum, or both) in the ground state. This classic "coherent state" dynamics is now very well known and is described in the next section.

By analogy to the 1-D case, we consider a harmonic crystal in its ground state with separable normal modes, disturbed by displacements of positions and momenta. We consider time-dependent Schrödinger oscillators for each normal-mode degree of freedom. This principle was previously used, for example, for a polyatomic molecule with 27 and 41 normal coordinates.[2]

Starting with a laboratory coordinate for each atom in a solid, which is supposed to be free floating, as on the space shuttle, we have $3N - 6$ internal, normal coordinates and 6 zero-frequency modes that arise from the translational and rotational symmetry of the whole.

2. COHERENT STATE DYNAMICS

The classic "coherent state" dynamics is now very well known; see, for example, ref 3. Specifically, for a harmonic oscillator with the Hamiltonian $H = p^2/2m + \frac{1}{2}m\omega^2 q^2$, a Gaussian wave packet beginning as

$$\psi(q, 0) = \exp\left[i\frac{A_0}{\hbar}(q - q_0)^2 + \frac{i}{\hbar}p_0(q - q_0) + \frac{i}{\hbar}s_0\right] \tag{1}$$

becomes, under time evolution

$$\psi(q, t) = \exp\left[i\frac{A_t}{\hbar}(q - q_t)^2 + \frac{i}{\hbar}p_t(q - q_t) + \frac{i}{\hbar}s_t\right] \tag{2}$$

where

$$\begin{aligned} p_t &= p_0\cos(\omega t) - m\omega q_0\sin(\omega t) \\ q_t &= q_0\cos(\omega t) + (p_0/m\omega)\sin(\omega t) \end{aligned} \tag{3}$$

(i.e., classical motion for the guiding trajectory (q_t, p_t)), and if $A_0 = im\omega/2$, then $A_t = A_0$. The phase then obeys

$$s_t = s_0 + \frac{1}{2}[p_t q_t - p_0 q_0 - \omega t] \tag{4}$$

More general "squeezed state" time-dependent solutions apply if the Gaussian spread of the initial wave packet is a narrower or broader Gaussian than is the ground state of the

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same oscillator. In this case, the Gaussian "breathes," becoming wider and narrower twice per period of the harmonic oscillator.

Arbitrary time-dependent harmonic potentials have exact solutions in terms of Gaussians and their parameters, which are always classical in nature. A more general propagation of time-dependent "excited state" Gaussians, that is, Hermite polynomials multiplying the Gaussians, can be defined.[4] Here we consider only the usual coherent state solutions.

Any imaginable classical motion of a harmonic solid must have a quantum analog, according to Schrödinger correspondence. Each normal mode of a finite crystal, no matter what the size, is a 1-D oscillator, with frequencies and "classical" parameters appropriate to the initial conditions. For example, below, we will consider the interesting events after an atom in a crystal is kicked by a γ-ray photon in the Mössbauer effect.

In the case of a Gaussian in a general, N-dimensional time-dependent quadratic form potential, the governing equations are[3]

$$\psi_t(\boldsymbol{q}) \equiv \psi_t(\boldsymbol{q}_t, \boldsymbol{p}_t; \boldsymbol{q}) = \exp\left[\frac{i}{\hbar}\{(\boldsymbol{q}-\boldsymbol{q}_t)\cdot\boldsymbol{A}_t\cdot(\boldsymbol{q}-\boldsymbol{q}_t) + \boldsymbol{p}_t\cdot(\boldsymbol{q}-\boldsymbol{q}_t) + s_t\}\right] \tag{5}$$

where $\boldsymbol{A}_t$ is an $N \times N$-dimensional matrix for N coordinates, and $\boldsymbol{q}$, $\boldsymbol{q}_t$, and $\boldsymbol{p}_t$ are N-dimensional vectors, which obey

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{q}_t = \nabla_p H \tag{6}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{p}_t = -\nabla_q H \tag{7}$$

$$\dot{\boldsymbol{A}}_t = -2\boldsymbol{A}_t^2/m - V''(q_t, t)/2 \tag{8}$$

By writing $\boldsymbol{A}_t$ in terms of two $N \times N$-dimensional matrices $\boldsymbol{P}_Z$ and $\boldsymbol{Z}$

$$\boldsymbol{A}_t = \frac{1}{2}\boldsymbol{P}_Z\cdot\boldsymbol{Z}^{-1} \tag{9}$$

with initial conditions satisfying $\boldsymbol{A}_0 = \frac{1}{2}\boldsymbol{P}_{Z_0}\cdot\boldsymbol{Z}_0^{-1}$, for example, $\boldsymbol{P}_{Z_0} = 2\boldsymbol{A}_0$ and $\boldsymbol{Z}_0 = \boldsymbol{I}$, eqs 8 and 4 become

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\boldsymbol{P}_Z\\ \boldsymbol{Z}\end{pmatrix} = \begin{pmatrix}0 & -\boldsymbol{V}''(t)\\ \boldsymbol{m}^{-1} & 0\end{pmatrix}\begin{pmatrix}\boldsymbol{P}_Z\\ \boldsymbol{Z}\end{pmatrix} \tag{10}$$

$$\dot{s}_t = L_t + \frac{i\hbar}{2}\mathrm{Tr}[\dot{\boldsymbol{Z}}\cdot\boldsymbol{Z}^{-1}] \tag{11}$$

or

$$s_t = s_0 + S_t + \frac{i\hbar}{2}\mathrm{Tr}[\ln \boldsymbol{Z}] \tag{12}$$

$\boldsymbol{V}''$ and $\boldsymbol{m}^{-1}$ are N-dimensional matrices of mixed second derivatives of the Hamiltonian with respect to position and momentum coordinates, respectively. That is

$$[\boldsymbol{V}'']_{ij} = \frac{\partial^2 H}{\partial q_i \partial q_j} \tag{13}$$

and so forth. Also

$$\begin{pmatrix}\boldsymbol{P}_{Z_t}\\ \boldsymbol{Z}_t\end{pmatrix} = \boldsymbol{M}(t)\begin{pmatrix}\boldsymbol{P}_{Z_0}\\ 1\end{pmatrix} \tag{14}$$

where from eqs 10 and 14, we have

$$\frac{\mathrm{d}\boldsymbol{M}(t)}{\mathrm{d}t} = \begin{pmatrix}0 & -\boldsymbol{V}''(t)\\ \boldsymbol{m}^{-1} & 0\end{pmatrix}\boldsymbol{M}(t) \tag{15}$$

$\boldsymbol{M}(t)$ is the stability matrix

$$\boldsymbol{M}(t) = \begin{pmatrix}\boldsymbol{m}_{11} & \boldsymbol{m}_{12}\\ \boldsymbol{m}_{21} & \boldsymbol{m}_{22}\end{pmatrix} \tag{16}$$

where $\boldsymbol{m}_{11} = \partial\boldsymbol{p}_t/\partial\boldsymbol{p}_0|_{q_0}$, $\boldsymbol{m}_{12} = \partial\boldsymbol{p}_t/\partial\boldsymbol{q}_0|_{p_0}$, $\boldsymbol{m}_{21} = \partial\boldsymbol{q}_t/\partial\boldsymbol{p}_0|_{q_0}$, and $\boldsymbol{m}_{22} = \partial\boldsymbol{q}_t/\partial\boldsymbol{q}_0|_{q_0}$.

3. PHONON MOMENTUM AND WAVE VECTOR

From the perspective of Schrödinger correspondence, the classical vibrational motion of a harmonic lattice and the motion of phonons must be more than analogous to each other; they must be derivable from one another. First, we need to understand the notion of a phonon, its mechanical momentum, and its pseudomomentum.

Ashcroft and Mermin[5] clarified the role of phonons by calling them corpuscles, stating, "Usually the language of normal modes is replaced by a corpuscular description...", and adding that the concept of a phonon is deliberately analogous to that of a photon. In his well-known textbook, Kittel[6] states "...a phonon really carries zero momentum..." Kittel was using the word "phonon" to mean a crystal normal mode, not a corpuscle, just as in quantum electrodynamics, where the word "photon" is sometimes used for a singly occupied cavity mode.

The understanding of phonon pseudomomentum versus mechanical momentum is star-crossed at best. The problem is traceable to the tradition of suppressing the role of whole crystal momentum, usually by eliminating it before eq 1, so to speak, by writing interactions in internal coordinates. Writing that pseudomomentum is sometimes called "crystal momentum", Kittel calls the momentum confusion a "delicate point" in a footnote, stating, "...Thus, in an H_2 molecule the internuclear vibrational coordinate $\boldsymbol{r}_1 - \boldsymbol{r}_2$ is a relative coordinate and does not carry linear momentum; the center-of-mass coordinate $(\boldsymbol{r}_1 + \boldsymbol{r}_2)/2$ corresponds to the uniform mode and can carry linear momentum."

Strangely, Kittel goes on to assign the "uniform mode" carrying momentum to the *internal* $K = 0$ phonon mode, that is, the infinite wavelength internal normal mode of a crystal. Because he, like almost all authorities, has long since abandoned the crystal center-of-mass translation, the $K = 0$ mode is the best thing left on the shelf, so to speak, but it is not correct. This mode only has the right flavor; the correct assignment is to the zero-frequency normal modes, an assignment that is correct even for a finite crystal. No internal mode can correctly describe the overall rigid translation of the crystal, which had just been highlighted by Kittel's H_2 example, which required only two atoms!

Nonetheless, Kittel clearly understands the essential momentum-carrying role of the center of mass. He did not assign a wave function to this mode, which is actually $\exp[i\vec{K}\cdot\vec{X}]$, where $\vec{X}$ is the center of mass of the crystal, for which $\vec{K} \neq 0$ in general. We call the momentum-carrying external modes "K" modes, in honor of Prof. Charles Kittel, age 102 as of this writing. We note that three rotational degrees of freedom are also K modes. It does not matter if the crystal is attached to a lab bench, and so on; momentum conservation is still maintained, and the attachment normally has no effect on internal crystal dynamics.

4. DEFINITIONS

We give some definitions that are desirable given the somewhat confusing statements that can be found in the literature. Even though the greater majority of sources are clear, enough "noise" exists to make this exercise worthwhile. Especially dangerous and confusing are loose statements about the manipulation of electron pseudomomentum by reciprocal lattice vectors. Phonon pseudomomentum is an entirely different matter.

It helps to put some objects in what we call the foreground, and the remainder of the whole crystal is the background. An electron or a phonon may be a foreground object, for example. A neutron passing through a crystal is a foreground object. Foreground objects may have mechanical momentum and pseudomomentum, which may or may not be preserved, and so, too, may the background. The momentum of the whole system, that is, the foreground plus the background, must be conserved.

The definitions given immediately below will be clarified by the linear and circular atom chains considered later.

The **mechanical linear momentum** of an object is defined classically as the sum of masses times the Cartesian velocities of the object's constituent particles and quantum mechanically as the sum over the particle momentum operators $-i\hbar\partial/\partial x_j$. The conservation of this momentum for the totality of objects is a consequence of the translational invariance of the total Hamiltonian. Similar statements are made about angular momentum. Any phonon mechanical momentum (there may or may not be any for a given phonon) is automatically assigned to the total crystal center-of-mass momentum by the definition of that momentum.

Phonon pseudomomentum $\vec{k}$ is a consequence of Hamiltonian symmetry under cyclic particle relabeling. Cyclic means that an atom at one face is reattached on an opposite face, in Born−von Karman fashion. This definition of phonon pseudomomentum differs from the usual crystal translation operator by primitive lattice vectors, which is problematic because the translation symmetry holds for any translation, not just by lattice vectors, and is really the symmetry of the total system momentum.

Phonon pseudomomentum will not be conserved if cyclic particle relabeling is not a symmetry, as when a defect is present, but it is conserved under phonon−phonon interactions induced by anharmonicity obeying crystal symmetries.

Taking an acoustic phonon mode as an example, the band edge amounts to alternate compression and expansion every unit cell. Any shorter wavelength oscillation does not exist physically and is equivalent to a longer wavelength oscillation obtained by adding a reciprocal lattice vector to bring the mathematically faster oscillation back into the physical Brillouin zone. See the Appendix for a discussion of phonon pseudomomentum.

Electron pseudomomentum is a consequence of Hamiltonian symmetry under electron translation by primitive lattice vectors *for a fixed crystal lattice*. The pseudomomentum acknowledges that mechanical momentum undulates for energy-conserving motion in a periodic potential. It is replaced by a pseudomomentum that is conserved.

Crystals have a pseudomomentum when they are considered a "background" object with an interior electron in the foreground. If the foreground object (electron) has pseudomomentum, then the background object (crystal) should have pseudomomentum. The symmetry leading to a crystal pseudomomentum is as follows: The electron is held fixed while the background is translated; an undulating potential is experienced, implying a background crystal pseudomomentum.

Total momentum results from translational symmetry of the whole system (both an electron and a crystal). The total momentum P is the sum of the electron pseudomomentum $\hbar k$ and crystal pseudomomentun $\hbar K$: $P = \hbar K + \hbar k$. This is especially apparent if the electron entered from outside the crystal: total mechanical momentum of crystal + electron is conserved, but the total momentum is the sum of two pseudomomenta while the electron is inside the crystal.

5. LINE OF ATOMS

Figure 2 begins the exercise of Schrödinger correspondence in an interesting many-body situation. We consider an N-atom

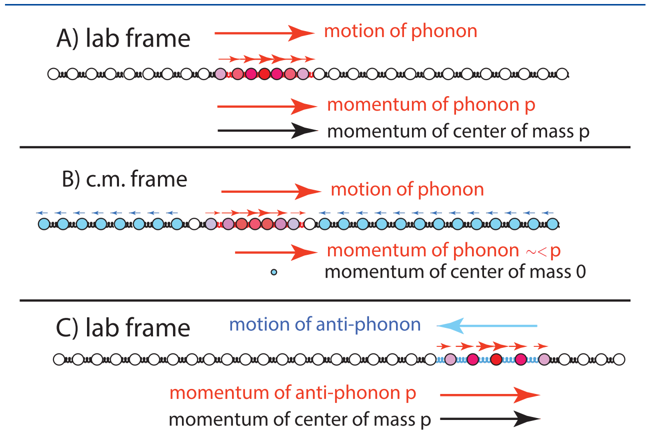

Figure 2. Three snapshots of a disturbance traveling in a linear chain of equal masses connected by equal force constants. Snapshot A is in the lab frame, B is in the center-of-mass frame at the same time as A, and C is taken later in the lab frame. Springs that are stretched relative to their equilibrium length are shown in blue, and those that are compressed are shown in red. Atoms moving right are red, and those moving left are blue, with saturation representing speed. The disturbance resulted from pushing the chain, initially at rest, from the left-end atom. See the text.

1D classical harmonic chain of atoms (1D crystal) and, by Schrödinger correspondence, a quantum chain. Such quasi-1-D chains are becoming experimentally realizable with dozens of atoms in a trap and are already the subject of dynamical investigations involving vibrational disturbances on the chain[7] and instabilities.[8]

The chain can be described in the laboratory or a center-of-mass frame. If the chain is initially at rest in the lab frame and the left-end atom is transiently forced left to right, then this causes a corpuscle of energy and momentum to travel down the chain. The system center-of-mass momentum will have received a boost. In Figure 2A,C, we describe the chain in the lab frame. The phonon corpuscle has a local momentum density traveling along the chain. Because atoms are not moving, except in the vicinity of the phonon, the center-of-mass momentum is entirely attributable to the phonon. It is often a matter of taste whether the momentum is thought of as belonging to the phonon or to the center of mass, but it should not be counted twice.

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Figure 2B shows motion in the center-of-mass frame. In the center-of-mass frame, the motion is entirely composed of "internal" normal modes, none of which has any momentum. A corpuscle (phonon) with locally demonstrable momentum is traveling from left to right, but atoms momentarily not participating in the phonon are drifting in the opposite direction, so as to make the total center-of-mass momentum vanish. Snapshots A and C are shown in the lab frame after the same push.

In panel C, we see the situation some moments after the phonon has reflected off the free right-hand end. A dilation has formed and is heading from right to left. Its momentum is opposite its direction of motion, and its mass density is below the average. The local momentum contained in the phonon has not changed. It is reasonably thought of as an antiphonon. Following the scenario of panels A and C, on average, over time, each mass drifts to the right, spending most of its time at rest, only to be rather suddenly displaced to the right as either the negative or positive mass density corpuscle passes by. Over time, the chain crawls to the right in an earthworm-like motion. By Schrödinger correspondence, we have just described the quantum-mechanical motion as well.

In the lab frame used in panels A and C, there is positive center-of-mass momentum carried by the K mode. All of this momentum is attributable to the corpuscle. This remains true after the corpuscle reflects from the end to become an anticorpuscle or antiphonon of lower-than-background mass density. The corpuscle's momentum still points to the right, now in opposition to its motion toward the left. Both before and after the collision with the free end, the corpuscle is responsible for the center-of-mass momentum, which cannot change in the absence of external forces. When the anticorpuscle collides with the left end, it again reflects as a corpuscle. The scenario corresponds roughly to an air pressure pulse in a tube with both ends open, apart from the part of the pulse that is radiated from the tube ends.

The foreground (corpuscle) momentum and the background momentum are different in the two frames. The corpuscle in B has a momentum slightly lower than that in panels A and C. This difference vanishes in the limit of a large chain because the drift velocity of the noncorpuscle masses is proportional to the inverse of the chain length. The time between passes of the corpuscle is proportional to the chain length. The displacement of atoms as the corpuscle passes by is independent of chain length. Over time, the atoms do not drift right or left in the center-of-mass frame.

The corpuscle in the lab frame chain has mechanical momentum, p, that can be calculated in the usual way by adding all of the velocities of the masses comprising it. If a large free mass is just touching the right-hand chain member, then very nearly (and exactly as the large mass approaches infinite mass), momentum $2p$ is imparted to the heavy mass as the corpuscle arrives (Figure 3). With the heavy mass present, the corpuscle now recoils as a positive mass density pulse, with reversed momentum. The heavy mass behaves just as if it had been struck elastically by a particle of momentum p, acquiring momentum $2p$. The total momentum of the chain plus heavy mass remains fixed.

If the chain is pushed to the right, followed quickly by an opposite pull, then a wave of compression, followed by rarefaction, is sent down the chain. The two parts together, if carefully balanced, have canceling, net-zero momentum, even though they may be traveling briskly down the chain. Energy is

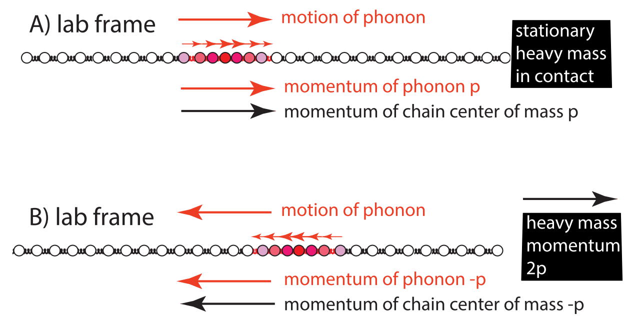

Figure 3. In panel A, the initial phonon in Figure 2 now heads toward a large stationary mass waiting in contact at the end of the chain. The mass imposes a nearly fixed boundary condition on the right-end atom, causing the reflection of a phonon in frame B with reversed momentum in the chain. The change in chain center-of-mass mechanical momentum, $-2p$, is balanced by the mechanical momentum gain $+2p$ of the heavy mass, showing that the phonon momentum was indeed real and of value p.

nonetheless being propagated in this composite phonon. The pushing and pulling could be done periodically, apart from fading in and out, creating a well-defined phonon pseudomomentum for a phonon with no mechanical momentum. Because of Schrödinger correspondence, we can take any classical scenarios quite seriously quantum mechanically. If so, we have learned that phonons can have mechanical momentum or not, quite apart from their pseudomomentum. We apply the Schrödinger correspondence explicitly to the ring of atoms considered next.

6. RING OF ATOMS

A chain of atoms connected to itself as in a circle (Born−von Karman boundary conditions) is a well-known model (Figure 4). Ashcroft and Mermin choose these conditions on an N-atom chain for convenience, stating, "for if N is large, and we are not interested in end effects, then the precise way in which the ends are treated is immaterial."[5] We disagree with this seemingly benign statement, for it hides once again the role of the total momentum or, here, the angular momentum. The zero-frequency angular momentum mode gets no mention in their treatment.

To be specific, an N-atom chain slides frictionlessly on a rigid ring confined to the plane. Each atom is linked by harmonic springs (Figure 4) to its neighbors.

Atoms with a clockwise drift are shown in light blue, and those with a counterclockwise drift are red. Atoms with a steady angle are white. On the left, the total angular momentum around the center of the ring vanishes, yet a corpuscle travels counterclockwise around the circle. The corpuscle has angular momentum if it is considered as a foreground object, with the momentum of atoms 12−17 added together. The background momentum cancels the foreground momentum, giving 0 total angular momentum. As the corpuscle passes each atom, the atom suddenly increases its angle counterclockwise; in between such times, the atoms slowly drift clockwise. Over time, there is no drift in angle. On the right, a component of the zero-frequency K mode (which here is the total angular momentum) has been added, just so as to cancel the clockwise drift in between arrivals of the corpuscle. The atoms make counterclockwise jumps, and, over time, steadily progress counterclockwise in angle. The progress of an atom with time in each case is shown at the bottom. On

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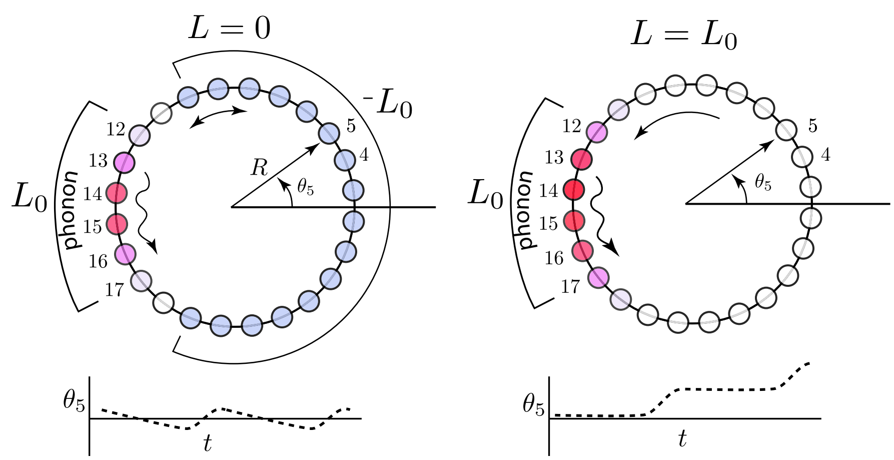

Figure 4. Ring of atoms linked by harmonic springs carries a phonon corpuscle with 0 angular momentum (left) or the angular momentum of the phonon (right). The angular progress of an atom over time is shown in each case at the bottom.

the left, the foreground corpuscle has angular momentum L_0, and the background has $-L_0$; total $L = 0$. This is a phonon corpuscle built out of states of 0 angular momentum. On the right, the compensated foreground corpuscle has angular momentum L_0, and the background has $L = 0$, with total angular momentum L_0.

We issue a warning that although this model has rotational symmetry and well-defined angular momentum, it has not been set free to flex or translate as a whole, so its physics is realistic only for 1D motion along the ring. If, for example, an atom in the ring was to emit a γ-ray into the 2D plane, then momentum would not be conserved.

We form N normal modes in the usual way. One of these modes has zero frequency or no restoring force. In that mode, all of the atoms move in unison around the ring. It is the only mode that can carry angular momentum.

The kinetic energy is that of N atoms, each of mass m, in a free-sliding heavy rigid ring of radius R. There are N angles required to specify the positions of the atoms, which interact by harmonic potentials with a Hamiltonian given as

$$H = \frac{1}{2mR^2}\sum_{l=1}^{N} L_l^2 + \sum_{l=1}^{N-1}\frac{1}{2}\kappa R^2(\theta_{l+1} - \theta_l)^2 \tag{17}$$

which is quantized as

$$H = -\frac{\hbar^2}{2mR^2}\sum_{l=1}^{N}\frac{\partial^2}{\partial\theta_l^2} + \sum_{l=1}^{N-1}\frac{1}{2}\kappa R^2(\theta_{l+1} - \theta_l)^2 \tag{18}$$

The normal modes χ_k that diagonalize the force matrix can be written down by symmetry, for N atoms on a ring of radius R, as

$$\chi_n = \frac{R}{\sqrt{N}}\sum_{l=1}^{N} e^{iak_n l}\theta_l = \frac{R}{\sqrt{N}}\sum_{l=1}^{N} e^{i2\pi nl/N}\theta_l \tag{19}$$

$$\theta_l = \frac{1}{R\sqrt{N}}\sum_{n=-b_N}^{b_N} e^{-iak_n l}\chi_n = \frac{1}{R\sqrt{N}}\sum_{n=-b_N}^{b_N} e^{-i2\pi nl/N}\chi_n \tag{20}$$

where n is $-(N-1)/2, ..., 0, ..., (N-1)/2$, $b_N = (N-1)/2$, $a = 2\pi R/N$, and $k_n = 2n\pi/Na$ with normal frequency $\omega_n = 2\sqrt{\kappa/m}\ \sin\left|\frac{k_n a}{2}\right| = 2\sqrt{\kappa/m}\ \sin\left|\frac{n\pi}{N}\right|$.

We wish to use real valued normal mode ξ_k. The χ_0 mode is already real, so we define $\xi_0 \equiv \chi_0$. We take two real linear combinations of the degenerate modes χ_n and χ_{-n} to make two standing waves, one a cosine, $\zeta_n = \frac{\chi_n + \chi_{-n}}{\sqrt{2}} = \frac{R}{\sqrt{N/2}}\sum_{l=1}^{N}\cos(2\pi nl/N)\theta_l$, where n is $[-b_N, -1]$, and one a sine, $\xi_n = \frac{\chi_n - \chi_{-n}}{\sqrt{2}i} = \frac{R}{\sqrt{N/2}}\sum_{l=1}^{N}\sin(2\pi nl/N)\theta_l$, where n is $[1, b_N]$. The Hamiltonian becomes, in the normal coordinates

$$H = \sum_{n=-b_N}^{b_N}\frac{1}{2m}p_{\xi_n}^2 + \sum_{n=b_N}^{b_N}\frac{1}{2}m\omega_n^2\xi_n^2 \tag{21}$$

with normal frequency $\omega_n = 2\sqrt{\kappa/m}\ \sin\left|\frac{k_n a}{2}\right| = 2\sqrt{\kappa/m}\ \sin\left|\frac{n\pi}{N}\right|$. The coordinate ξ_0 stands out as having no restoring force. It is the K mode, a measure of the overall rotation of the atoms of the ring; its conjugate momentum is proportional to the angular momentum.

Classically, the total angular momentum reads

$$L = \sum_{l=1}^{N} mR^2\dot{\theta}_l = \sqrt{N}mR\dot{\xi}_0 \equiv MR^2\dot{\Theta} \tag{22}$$

and $M = \sum_l m$ and $\Theta = \sum_l \theta_l/N$. The angular momentum of the ring is the sum of the angular momenta of the atoms. The angular momentum operator for the ring of N atoms with angle θ_l and of mass m and a ring of radius R is

$$\hat{L} = \sum_{l=1}^{N}\hat{L}_l = -i\hbar\sum_{l=1}^{N}\frac{\partial}{\partial\theta_l} = -i\hbar\frac{\partial}{\partial\Theta} \tag{23}$$

To quantize this system, we take the Hamiltonian in normal coordinates (for N odd)

$$H = -\sum_{n=b_N}^{b_N}\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\xi_n^2} + \sum_{n=b_N}^{b_N}\frac{1}{2}m\omega_n^2\xi_n^2 \tag{24}$$

where

$$\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\xi_0^2} = \frac{\hbar^2}{2MR^2}\frac{\partial^2}{\partial\Theta^2}$$

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An eigenstate of the chain reads, with angular momentum $\hbar K$ in the (zero-frequency) rotational mode, η_n quanta in the nth mode, and so on

$$|K, \boldsymbol{\eta}\rangle = e^{iK\Theta} \prod_{\substack{n=-b_N \\ n\neq 0}}^{b_N} |\eta_n\rangle \tag{25}$$

where

$$\langle \xi_n|\eta_n\rangle = \frac{1}{\sqrt{2^{\eta_n}\eta_n!}}\left(\frac{m\omega_n}{\pi\hbar}\right)^{1/4} e^{-m\omega_n\xi_n^2/2\hbar} H_{\eta_n}\left(\sqrt{\frac{m\omega_n}{\hbar}}\,\xi_n\right) \tag{26}$$

Any $\eta_n = 1$ means a singly occupied normal mode. (We are reserving the term "phonon" for corpuscles, as per standard usage.) The angular momentum $\hbar K$ with K as an integer owes its existence to the K-mode free rotation, independent of the normal modes, which carry no momentum. This is obvious if we apply the total angular momentum operator $\hat{L} = -i\hbar\partial/\partial\Theta$ to the wave function of eq 25; we get $\hbar K$, independent of the internal normal-mode quantum numbers. Because the function must be the same for Θ and $\Theta + 2\pi$, K must be an integer, and the angular momentum is quantized to $L = \hbar K$. The occupation of any phonon of coordinate ξ_n and wavenumber k_n, where $n \neq 0$, contributes no angular momentum, that is, no mechanical momentum, despite superficial appearances (eq 19).

We are not particularly interested in the restriction of allowable angular momenta due to the finite number N of atoms in the ring. Rather we take the macroscopic limit of a huge moment of inertia and large N. Then angular momentum becomes, in effect, a continuum, and we approach the idealization of a large crystal.

There are several ways to make a spatially localized phonon wave packet. Perhaps the simplest is to use Schrödinger correspondence. Starting with a 0 K ground state

$$|0, \mathbf{0}\rangle = e^{i0\Theta} \prod_{n=-b_N}^{b_N} |0_n\rangle \tag{27}$$

we apply a momentum boost to a group of adjacent atoms of the form

$$e^{\sum_l ip_l\theta_l/\hbar}$$

imparting angular momentum $p_l = \hbar K\nu\cdot\exp\left[-\alpha(l-l_0)^2\right]$ to the lth atom, creating

$$|\psi_{\text{boost}}\rangle = e^{\sum_l ip_l\theta_l/\hbar}|0, \mathbf{0}\rangle = e^{iK\Theta}\sum_{\boldsymbol{\eta}} a_{\boldsymbol{\eta}}|\boldsymbol{\eta}\rangle \tag{28}$$

where $|\boldsymbol{\eta}\rangle$ is shorthand for

$$|\boldsymbol{\eta}\rangle = \prod_{\substack{n=-b_N \\ n\neq 0}}^{b_N} |\eta_n\rangle$$

The parameter ν is chosen so that $\sum_l p_l = \hbar K$. The boosted state imparts momentum to each atom, maximizing at the atom $l = l_0$. The angular momentum imparted to the center of mass is definite

$$\hat{L}|\psi_{\text{boost}}\rangle = \hbar K|\psi_{\text{boost}}\rangle$$

The situation just described corresponds to Figure 4, right. A group of atoms has been given a real, mechanical momentum and, collectively, they have contributed to the total (mechanical) angular momentum.

Phonon Momentum. In building a localized phonon, any mechanical momentum it possesses accrues to the center-of-mass momentum or angular momentum. However, there is a practical sense in which the momentum may be associated with the phonon itself. Indeed, we have just created a phonon with mechanical momentum that is attributable to a local disturbance.

The local phonon's effect on the total angular momentum of the ring can be canceled by applying a reverse boost, that is

$$e^{-iK\Theta}|\psi_{\text{boost}}\rangle = e^{-iK\Theta}e^{\sum_l ip_l\theta_l/\hbar}|0, \mathbf{0}\rangle = \sum_{\boldsymbol{\eta}} a_{\boldsymbol{\eta}}|\boldsymbol{\eta}\rangle \tag{29}$$

This wave function has no total momentum, but atom-by-atom inspection with the operators

$$\hat{p}_l = -i\hbar\frac{\partial}{\partial\theta_l}$$

reveals a group of atoms near $l = l_0$ with collective net momentum. The sum over all atoms gives zero momentum. This exactly corresponds to Figure 4, left.

The phonon in Figure 4 does not have a very well-defined pseudomomentum because it is a pulse with no modulation.

Phonon Pseudomomentum. How can a spatially localized phonon be created, with a well-defined pseudomomentum, near the atom labeled by l_0? We can use a linear superposition of one quantum normal mode of nearby k_n, a narrow range of states of nearby pseudomomentum. We will create a state with no total angular momentum (because angular momentum is conserved, and none of the normal modes have any) but well-defined pseudomomentum.

Apart from normalization, we take

$$|\psi_{n,\alpha,l_0}(\boldsymbol{\xi})\rangle \approx \sum_m e^{-(1/2\alpha)(m-n)^2 - ik_m a l_0}|0\rangle|0\rangle\ldots|1_m\rangle|0\rangle\ldots|0\rangle \tag{30}$$

or

$$\psi_{n,\alpha,l_0}(\boldsymbol{\xi}) \approx \left(\sum_m e^{-(1/2\alpha)(m-n)^2 - ik_m l_0}\xi_m\right)e^{-\sum_{n'} m\omega_{n'}\xi_{n'}^2/2\hbar}$$
$$\equiv \xi_{n,\alpha,l_0}e^{-\sum_{n'} m\omega_{n'}\xi_{n'}^2/2\hbar} \tag{31}$$

The parameter k_n controls the average pseudomomentum of the result; the phonon is centered on the site l_0. The result is described as

$$\xi_{n,\alpha,l_0} \approx \frac{R}{\sqrt{N}}\sum_{l=1}^{N} e^{ik_n a(l-l_0) - (\alpha/2)(l-l_0)^2}\theta_l \tag{32}$$

which leaves atoms with labels far from l_0 unaltered but acts like ξ_n near $l = l_0$. ξ_{n,α,l_0} is a compromise between Fourier extremes of fixed position and fixed wave vector. This phonon involves only singly occupied normal modes by construction.

Phonon–Phonon Interaction. Because there is no real mechanical momentum associated with the pseudomomentum, there is no concern about momentum conservation when phonons interact due to anharmonicities or impurities. Energy must be conserved in any case. For anharmonicities that are uniform throughout the crystal and intrinsic to the atomic interactions, cyclic atom replacement symmetry exists, and total pseudomomentum conservation applies. For example, if the energy dispersion is sufficiently linear in the long wavelength acoustic region, then two phonons may interact anharmonically to give two new phonons

$$k_n + k_{n'} \rightarrow k_m + k_{m'}$$

where $n + n' = m + m'$.

7. TIME EVOLUTION OF A MÖSSBAUER-LIKE KICK

The showpiece of many-body elastic quantum transitions is certainly Mössbauer emission, which features a demonstrably purely elastic component: No internal lattice phonon occupations change in a large block of material, despite a sharp kick to one of its atoms. Only the K mode is affected in this fraction of elastic events.

The sample mass is normally so large that the energy (due to momentum conservation) exchanged in a zero-phonon process is truly infinitesimal. A sample of the nuclear ground state of ^{57}Fe placed nearby will hungrily soak up any such γ-ray with an enormous resonant cross section. So narrow is the Mössbauer line that moving the nearby sample at a centimeter per second or less relative to the emitter can Doppler shift the resonance absorption line more than its intrinsic line width and let the radiation pass through the sample unhindered, as detected by a counter. There can be little doubt: Some of the emission is totally elastic; it is not just "quasi-elastic". The theory of Mössbauer emission[9] verifies this conclusion.

The remainder of the γ-ray emission by the same nucleus in the same surroundings gives a broad continuum of mostly lower energy due to phonon production for cold samples. Warmer samples also reveal phonon destruction events. Each emission event, whether totally elastic or not, must be accompanied by recoil of the sample with exactly the opposite momentum of the γ-ray. There is no escape from whole sample recoil even if phonons are created in the emission. Phonon momentum simply and instantly adds to the sample bulk momentum, as discussed above.

The beginnings (although not a proof) of the quantum effect responsible for the ultranarrow Mössbauer line can be seen in a 1-D oscillator, essentially an Einstein model of a solid (Figure 5). A quantum coherent state wave packet unquestionably oscillates in classical fashion (i.e., Schrödinger correspondence) after a kick due to γ-ray emission. However, if the wave packet energy is measured, then it may be found to be lying quietly in its ground state. The cross section for resonant reabsorption by another nearby ^{57}Fe is large, and within about a nanosecond, the energy of the γ-ray (and thus the lattice energy change) can me measured.

The spectrum of energies of the γ-rays looks like that in Figure 6, left. Discussions of "Mössbauer spectroscopy" often summarize this beautiful physics only briefly and rather tend to focus on something admittedly more practical: the technique of using tiny shifts of the nuclear resonance energy to probe the chemical environments of the unstable nucleus. This is detected (Figure 6) by shifts in the resonant Doppler speeds often well under centimeters per second and possible multiple resonance lines. The shifts reflect electric and magnetic field effects on the nuclear energy level, modulated again by the surroundings of the nucleus and therefore a very useful probe. This is the business end of Mössbauer spectroscopy, and it deserves the attention it gets. But for present purposes, it is the phonon-less recoil that concerns us. This recoil can involve any of the six degrees of freedom of zero-frequency K modes.

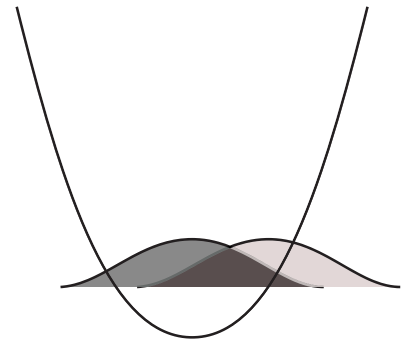

Figure 5. Ground-state Gaussian quantum eigenstate of the harmonic oscillator on the left, centered in the potential, is displaced in position, as shown with the lighter colored Gaussian displaced to the right. The Gaussian has indeed been displaced. Under time evolution, it will oscillate back and forth classically (Schrödinger correspondence). But suppose we ask, "What is the probability that the displaced Gaussian is still in the undisturbed ground state?" The overlap between the two states shows that this probability is significant, even though classically the function has been displaced with certainty.

In addition to the ultranarrow phonon-less Mössbauer line, there is a broad continuum of γ-ray emission that is of lower energy because a phonon (or more than one) has been deposited in the crystal. If so, there are internal agents set loose in the crystal, a phonon or phonons. Again, the whole crystal momentum has jumped by an equal and opposite amount to the γ-ray. That amount is slightly lower in magnitude for the inelastic component; the γ-ray is slightly lower frequency if phonons have been created.

The wave vector of the momentum to be deposited is ~70 Å^{-1}. This is usually deposited into total crystal recoil without a phonon being created or destroyed, that is, the Mössbauser line. If a phonon is created, then it need not be responsible for all of the recoil momentum. Indeed, the momentum can be divided between background recoil and phonons (if we choose to put them in the foreground), the sum of which is total system recoil momentum, which is exactly equal and opposite to the photon momentum, now very slightly reduced due to the energy deposited in phonons.

The Mössbauer effect continues to surprise. For example, a clever way of partitioning the γ-ray emission into pulses was proposed in ref 11.

The proper derivation of the Mössbauer γ-ray spectrum is given by Maradudin.[9] Here we will examine an ersatz Mössbauer kick (Figure 7) by providing an instantaneous momentum boost to a single atom. The exact momentum supplied to the system is therefore given, whereas it varies somewhat in γ-ray emission according to whether a phonon or phonons accompany the emission.

An impulsive kick to one atom (as in Mössbauer γ-ray emission) in a harmonic chain produces a phonon–antiphonon pair, seen in Figure 7 propagating in five snapshots at increasing times. The motion is indicated by red atoms if it is traveling right to left, by red springs if the springs are compressed relative to equilibrium, and by blue springs if they are extended. At the top, the mth atom has just been accelerated (kicked), but there is no displacement as yet. In step 2, the atom to its left has been accelerated and moved slightly, and the atom to its right has been pulled to the left.

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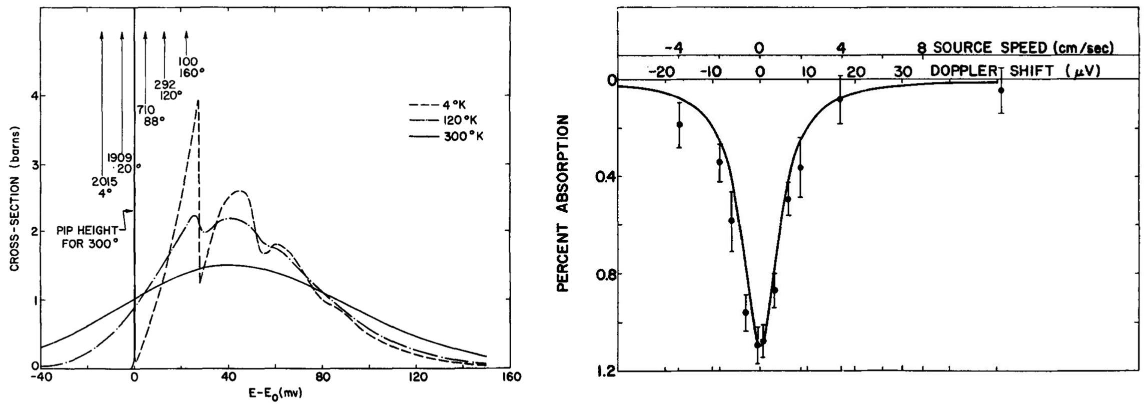

Figure 6. (left) A figure like this one from 1960 showing the Mössbauer line as an ultranarrow "pip" on a much broader background[10] is very hard to find under the heading of Mössbauer emission, even with a broad Wikipedia search. The pip height is given as a function of temperature; note that it is ~500 times taller than the ordinate of the graph at 4 K. It is often the case that "Mössbauer spectroscopy" is discussed even in a pedagogical article without beginning with a figure like the one on the left showing what is really going on. Almost universally, Mössbauer spectroscopy and even the more fundamental "Mössbauer effect" are shown only as on the right, spectra that are unremarkable to the eye, unless you notice the x axis labeled in Doppler shifts at speeds of centimeters per second. Reprinted with permission of ref 10. Copyright 1960 Elsevier.

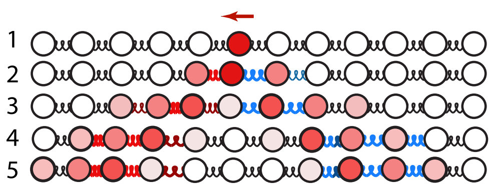

Figure 7. Phonon−antiphonon pair is created by a Mössbauer-like kick.

This sets up a cascading propagation of disturbances in both directions. A dilation can be seen heading to the right, and a compression is seen heading to the left. Both the phonon and the antiphonon have right-to-left momentum with atoms moving to the left as either disturbance passes by. In this scenario, the atoms become permanently displaced. By the Schödinger correspondence, this scenario has direct quantum counterparts. This figure omits rapid local back-and-forth oscillation with no momentum-transfer consequences; see Figure 8. Suppose $\psi_{n,\alpha,\theta_0}(\boldsymbol{\xi})$ is a lattice that just got a momentum kick $\hbar k$ to an atom at position l_m. What happens under time evolution? We take phonons to be absent initially and suppose no initial center-of-mass momentum. The initial many-body wave function is then (apart from normalization)

$$\psi(\boldsymbol{\xi}, 0) = e^{-\sum_n m\omega_n \xi_n^2/2\hbar} \tag{33}$$

Each ground-state normal mode simply evolves with a phase factor appropriate to its energy, but all of these phase factors add in the exponent, and nothing but an overall phase develops. This is another way to say that the ground state is stationary. After the lth atom gets its kick at $t = 0$, it becomes

$$\psi_{lk}(\boldsymbol{\xi}, 0) = e^{-\sum_n m\omega_n \xi_n^2/2\hbar} e^{ikR\theta_l} \tag{34}$$

We can ask the following questions now and as time evolves:

(1) What is the momentum of the center of mass?
(2) What is the time evolution of the many-body wave function?
(3) Where is the momentum located on the chain?
(4) What is the probability that the kick produced no phonons (i.e., was elastic)?
(5) What is the distribution of other phonon probabilities?

Only the answers to (2) and (3) will depend on time if the system is not further disturbed. We now address these questions in turn.

(1) The momentum delivered to one atom was $\hbar k$. Because there was no center-of-mass momentum to begin with, we had better find that the momentum of the center of mass is now also $\hbar k$. The atom with coordinate θ_{l_0} is expanded as

$$\theta_l = \sum_{n=0}^{N-1} U_{ln}\xi_n = \frac{1}{R\sqrt{N}}\xi_0 + \sum_{n=1}^{N-1} U_{ln}\xi_n \tag{35}$$

where $\xi_0 = \frac{R}{\sqrt{N}}\sum_{j=1}^{N}\theta_j$ The center-of-mass coordinate for N identical masses along a line at positions θ_j is

$$\Theta = \frac{1}{N}\sum_{j=1}^{N}\theta_j = \frac{1}{R\sqrt{N}}\xi_0 \tag{36}$$

The wave function eq 34 at $t = 0$ with the kick $e^{ikR\theta_l}$ has the term $e^{ik(1/\sqrt{N})\xi_0} = e^{ik\Theta}$, proving that the center of mass acquired the correct momentum.

(2) To find the time evolution of the many-body system, we use Schrödinger correspondence and the equations

$$\begin{aligned} \xi_{nt} &= \frac{\hbar k_n}{m\omega_n}\sin\omega_n t \\ p_{nt} &= \hbar k_n \cos(\omega_n t) \end{aligned} \tag{37}$$

where $k_n = kU_{ln}$ and the wave function evolves as

$$\psi_{lk}(\boldsymbol{\xi}, t) = e^{-\sum_n m\omega_n(\xi_n - \xi_{nt})^2/2\hbar + ip_{nt}(\xi_n - \xi_{nt})/\hbar + i\phi_t} \tag{38}$$

We will not bother to specify the overall phase here.

(3) To ask where in the chain the momentum density lies, we need to examine the atomic momentum operators

$$\hat{p}_j = -i\hbar\frac{1}{R}\frac{\partial}{\partial\theta_j} \tag{39}$$

At $t = 0$, eq 34 reveals, of course, that the (real) momentum resides locally on the lth atom. We want to discuss the situation as time evolves.

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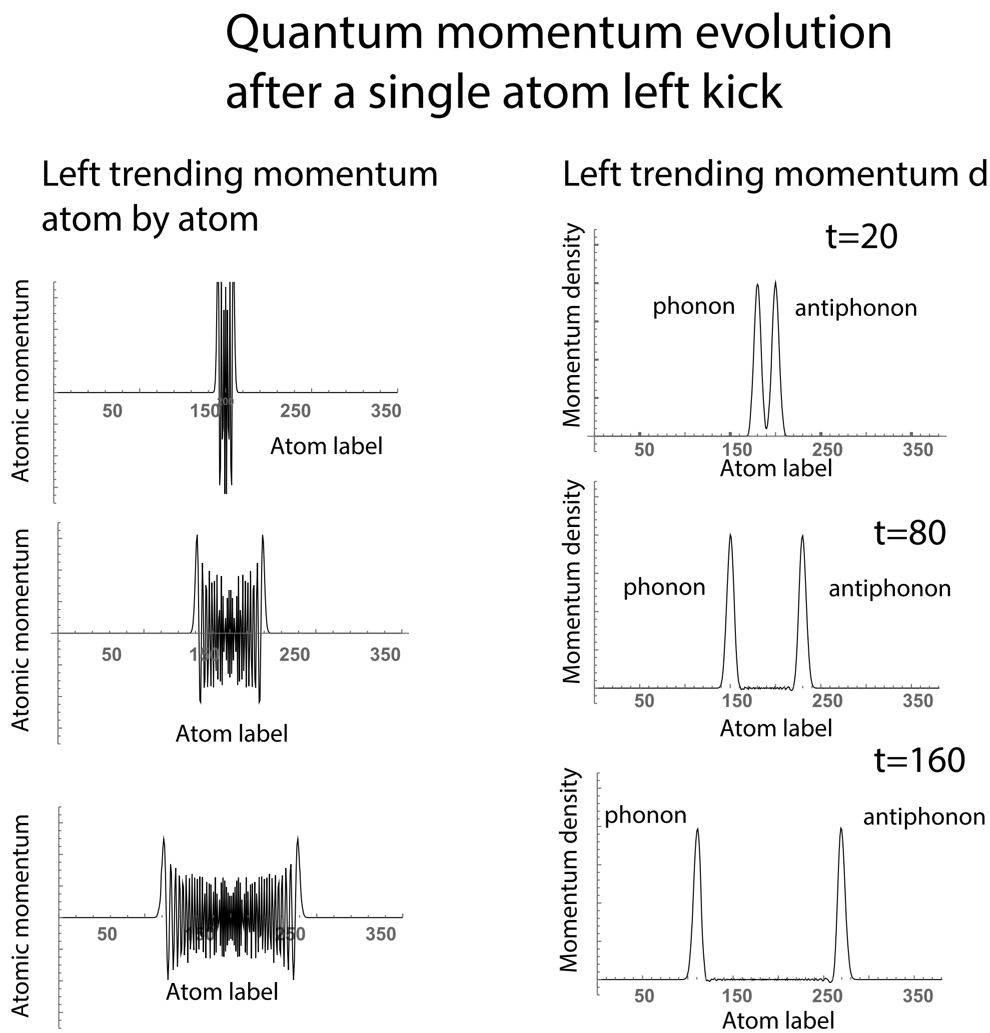

Figure 8. Here the central atom was kicked to the left, and the positive values in the plots are left-heading momenta.

We apply the momentum operator for each atom separately and plot the results atom-by-atom (Figure 8, left column) or averaged over a range of neighboring atoms (Figure 8, right column) to get a momentum density. Here the central atom was kicked to the left, and the positive values are left-heading momenta. Note that the phonon−antiphonon narrative is confirmed. This is not a semiclassical result of some sort; by Schrödinger correspondence, it is the exact result. The group velocity of the phonon is $v_g \approx \delta\omega/\delta k \approx a\sqrt{\kappa/m}$ at long wavelengths.

Schrödinger correspondence and the classical mechanics of the chain inform us that the kick produces a phonon−antiphonon pair (Figure 7). The phonon and the antiphonon travel in opposite directions, departing the site of the kick but carrying the same momentum. This is certainly different than the standard picture of a "phonon" heading off in one direction, carrying all of the momentum. The classical reason for the pair production is clear from Figure 7, and by Schrödinger correspondence, it is clear that the classical picture is extremely relevant to the quantum evolution.

(4) What is the probability that the kick produced no phonons? This is given by the square amplitude, in the case of an initial quiescent ring, as

$$\begin{aligned} P_{\mathrm{elastic}} &= |\langle\psi_0(\boldsymbol{\xi})|e^{ikR\theta_l}|\psi_0(\boldsymbol{\xi})\rangle|^2 \\ &= \left|R^N \int \mathrm{d}\theta_l\, e^{ikR\theta_l}\cdot \int \mathrm{d}\theta_1 \dots \mathrm{d}\theta_{l-1}\, \mathrm{d}\theta_{l+1} \dots \langle\psi_0(\boldsymbol{\xi})|\psi_0(\boldsymbol{\xi})\rangle\right|^2 \\ &= \left|R \int \mathrm{d}\theta_l \sqrt{\frac{w}{\pi}}\, e^{ikR\theta_l} e^{-wR^2\theta_l^2}\right|^2 \\ &= e^{-k^2/2w} \equiv e^{-2W} \end{aligned} \tag{40}$$

The elastic fraction e^{-2W} is called a Debye−Waller factor and is clearly related to the root-mean-square dispersion of the impacted atom. This result carries over to finite temperature. The finite elastic fraction for Mössbauer emission in a 3-D solid at finite temperature is affirmed by the fact that subangstrom resolution of atoms in scanning tunneling microscopy scans of surfaces is possible. It would not be if the root-mean-squared position dispersion of an atom was large.

(5) The elastic zero-phonon line is flanked by a density of inelastic processes that have an energy spectrum given by the Fourier transform of the autocorrelation of the kicked state

$$\Sigma(\omega) = \int \mathrm{d}t\; e^{i\omega t}\langle\phi|\phi(t)\rangle \tag{41}$$

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where $|\phi\rangle = e^{ikR\theta_l}|\psi_0(\xi)\rangle$ and $|\phi(t)\rangle = e^{-iHt/\hbar}|\phi\rangle$. The autocorrelation $\langle\phi|\phi(t)\rangle$ is evaluated using eq 38 and straightforward Gaussian integrals, but its Fourier transform is problematic, and it is best evaluated numerically.

8. CONCLUSIONS

The Schrödinger Correspondence Principle is a useful tool to understand the various aspects of harmonic solids by converting quantum-mechanical problems to classical ones. The clear (corpuscular) definition of a phonon, the importance of taking into account the center-of-mass momentum, and the concept of antiphonon are explained through the examples of the line and ring of atoms. The quantum behavior of harmonic solids under a Mössbauer-like kick is analyzed classically, verifying the existence of antiphonon through the simulation. Beyond the examples of this Article, we expect the Schrödinger Correspondence Principle to be useful in understanding anharmonic interactions, electron−phonon interactions, and other fundamental processes in solids.

APPENDIX: SYMMETRY AND PHONON PSEUDOMOMENTUM

What symmetry gives rise to phonon pseudomomentum? It is not best thought of as a translational symmetry. Continuous translational symmetry gives rise to ordinary total momentum and is a symmetry possessed by a finite crystal residing in free space. The system Hamiltonian is the same under any free translation; it gives rise to system center-of-mass momentum conservation. The translation of the system that happens to be by a lattice translation vector is nothing special; the Hamiltonian is the same even if the translation is not a lattice vector. Classical particle shift symmetry is a more appropriate symmetry: We replace atoms with their neighbors in a toroidal geometry, as in $x_n \to x_{n+1}$, with $x_N \to x_1$.

For a circular ring of identical atoms with identical forces between them, labeled by their angle θ_i on the ring, the invariance of Hamiltonian under the operator $\mathcal{R}_+$ can be written

$$\mathcal{R}_+H(\theta_1, \theta_2, ..., \theta_N) = H(\theta_N, \theta_1, ..., \theta_{N-1})\mathcal{R}_+ = H(\theta_1, \theta_2, ..., \theta_N)\mathcal{R}_+$$

that is, $\theta_i \to \theta_{i-1}$ and $\mathcal{R}_+H = H\mathcal{R}_+$. There is also the inverse operator with the reverse replacement and a finite cyclic group. This is a permutation symmetry of labels, after which operation the Hamiltonian reads the same. Cyclic atom replacement requiring $\mathcal{R}_+H = H\mathcal{R}_+$ is certainly not a continuous translation symmetry, and it cannot generate a traditional momentum. The Schrödinger equation satisfies

$$\mathcal{R}_+H\mathcal{R}_+^{-1}\mathcal{R}_+\psi(\chi) = H[\mathcal{R}_+\psi(\chi)] = E[\mathcal{R}_+\psi(\chi)] \tag{42}$$

with $\chi = (\theta_1, \theta_2, ..., \theta_N)$, which implies that eigenfunctions of H are or can be chosen (if they are degenerate) to be eigenfunctions of $\mathcal{R}_+$. With the mod N condition

$$\mathcal{R}_+^p\psi(\chi) = e^{ipk_m a}\psi(\chi) \tag{43}$$

where m and p are integers, which implies a pseudomomentum $k_m = 2\pi m/Na$, where a is the distance between neighbors.

However, this momentum is only defined within multiples of a reciprocal lattice vector because $k_m \to k_m + 2\pi M/a$ does not change the phase factor $e^{ik_m a}$. Thus, in any manipulations, we may want to adjust k to put it in the first Brillouin zone by adding multiples of reciprocal lattice vectors. This is optional because other Brillouin zones are just copies of the first one.

If some atoms or bonds differ in some way, then $\mathcal{R}_+H \neq H\mathcal{R}_+$ and the atom shift symmetry is broken. The phonon wave vector or pseudomomentum will not be conserved.

The conservation of phonon pseudomomentum for a collection of phonons works like the conservation of mechanical momentum: The sum of the momenta must be conserved, although individual momenta may change if the crystal is anharmonic, causing phonons to interact.

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Notes

The authors declare no competing financial interest.

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