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Phonon dynamics

(emission/lattice)

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ABSTRACT **An atomic lattice in its ground state is excited by the rapid displacement and release of an atomic constituent. The time dependence of the energy transfer to other constituents is studied by using a phonon dispersion relation that is linear in frequency and propagation vector components.**

The small-amplitude vibrations of an atomic lattice are customarily described in terms of nonlocal phonon excitations. With the simplification of three-dimensionally degenerate modes, labeled ϕ, the Hamiltonian for this description is

$$\mathcal{H} = \sum_{\phi} \hbar\omega_\phi \mathbf{y}_\phi^\dagger \cdot \mathbf{y}_\phi. \qquad [1]$$

Exhibited here for each mode are the single phonon energy $\hbar\omega$, the phonon annihilation operator $\mathbf{y}$, and the adjoint creation operator $\mathbf{y}^\dagger$, which operators form the phonon number operator for the degenerate mode: $\mathbf{y}^\dagger \cdot \mathbf{y}$.

An alternative description refers to the N localized constituents of the lattice, which are labeled $a, \ldots$ This version of the Hamiltonian for constituents of mass M, which uses coordinates $\mathbf{r}_a$ and momenta $\mathbf{p}_a$, is (1)

$$\mathcal{H} = \sum_a \frac{\mathbf{p}_a^2}{2M} + \sum_{ab} \frac{M}{2} (\mathbf{r} - \mathbf{r}_0)_a \cdot \Omega_{ab}^2 (\mathbf{r} - \mathbf{r}_0)_b - \sum_a \frac{3}{2} \hbar\langle\omega\rangle. \qquad [2]$$

Here, $\langle\,\rangle$ symbolizes the average over the phonon spectrum, and

$$\Omega_{ab}^2 = \langle \omega^2 e^{i\mathbf{k}\cdot(\mathbf{r}_{0a} - \mathbf{r}_{0b})} \rangle \equiv \frac{1}{N} \sum_\phi \omega_\phi^2 e^{i\mathbf{k}_\phi\cdot(\mathbf{r}_{0a} - \mathbf{r}_{0b})}, \qquad [3]$$

in which $\mathbf{k}$ is a mode propagation vector. The definition of the $N \times N$ matrix Ω^2 is extended to Ω^n, $n = -1, 0, 1, \ldots$, by the corresponding introduction of ω^n.

The equations of motion about the equilibrium positions $\mathbf{r}_{0a}$ are given, in matrix notation, by

$$M \frac{d}{dt} \mathbf{r}(t) = \mathbf{p}(t)$$

and

$$-\frac{d}{dt} \mathbf{p}(t) = M\Omega^2[\mathbf{r}(t) - \mathbf{r}_0]. \qquad [4]$$

The solutions, relating time t to time 0, are

$$(\mathbf{r} - \mathbf{r}_0)(t) = \cos \Omega t\, (\mathbf{r} - \mathbf{r}_0)(0) + \frac{1}{M} \frac{\sin \Omega t}{\Omega} \mathbf{p}(0)$$

and

$$\mathbf{p}(t) = \cos \Omega t\, \mathbf{p}(0) - M\Omega \sin \Omega t\, (\mathbf{r} - \mathbf{r}_0)(0). \qquad [5]$$

Consider a lattice in its phonon vacuum state. At time 0 the system is disturbed by singling out a particular mass, labeled α, which is abruptly removed from the neighborhood of its equilibrium position, $\mathbf{r}_{0\alpha} = 0$, given the displacement $\mathbf{D}$, and released. How does the energy thus imparted to the system spread out into the lattice?

For mathematical simplicity, D is taken to be large on the scale of vacuum fluctuations. (That such a D need not be in the small amplitude range is duly noted and deferred for later study.) According to Eqs. **2** and **3**, the energy initially fed into the α constituent is

$$E = \frac{1}{2} MD^2 \langle \omega^2 \rangle. \qquad [6]$$

How much energy is still so localized at a later time t?

One learns from Eq. **5** that, at the D level,

$$(\mathbf{r} - \mathbf{r}_0)(t)_\alpha = \mathbf{D}(\cos \Omega t)_{\alpha\alpha} = \mathbf{D}\langle \cos \omega t \rangle$$

and

$$\mathbf{p}(t)_\alpha = -M\mathbf{D}(\Omega \sin \Omega t)_{\alpha\alpha} = M\mathbf{D} \frac{d}{dt} \langle \cos \omega t \rangle, \qquad [7]$$

which says that

$$E_\alpha(t) = \frac{1}{2} MD^2 \left[\left(\frac{d}{dt} \langle \cos \omega t \rangle \right)^2 + \langle \omega^2 \rangle \langle \cos \omega t \rangle^2 \right]. \qquad [8]$$

The small-t behavior is conveyed by

$$E_\alpha(t)/E \cong 1 - \frac{1}{4} t^4 (\langle \omega^4 \rangle - \langle \omega^2 \rangle^2), \qquad [9]$$

and one sees the initial phase of a general property: there is no time dependence with a monochromatic spectrum. This, of course, is expected physically because that limit is the Einstein model of uncoupled oscillators.

One might try to move away from the Einstein model by assuming a narrow Lorentzian spectrum ($\delta\omega << \langle\omega\rangle$):

$$\langle f(\omega) \rangle_{\mathrm{L}} = \int d\omega\, f(\omega) \frac{\frac{1}{2\pi}\delta\omega}{(\omega - \langle\omega\rangle)^2 + \left(\frac{1}{2}\delta\omega\right)^2}. \qquad [10]$$

For application to Eq. **8**, one notes that

$$\langle \cos \omega t \rangle_{\mathrm{L}} = e^{-\delta\omega t/2} \cos\langle\omega\rangle t. \qquad [11]$$

Then, if $\langle\omega\rangle^2$ is effectively identified with $\langle\omega^2\rangle$, the familiar exponential decay emerges,

$$E_\alpha(t)/E = e^{-\delta\omega t}. \qquad [12]$$

That the short-time behavior in Eq. **12** does not agree with Eq. **9** traces back to the nonexistence of the Lorentzian averages, $\langle\omega^4\rangle_L$ and $\langle\omega^2\rangle_L$.

For a more physical—and yet mathematically simple—model, consider the dispersion relation

$$\omega_\phi = \underline{\omega} + u(|k_x| + |k_y| + |k_z|)_\phi, \qquad [13]$$

which has the separation property

$$e^{-i\omega_\phi t} = e^{-i\underline{\omega}t}\prod_{xyz} e^{-iu|k|_\phi t} \qquad [14]$$

and permits explicit evaluation of the spectral average.

Let each one-dimensional k spectrum be

$$k_m = \frac{2\pi}{a}\frac{m}{\nu}, \qquad m = 0, \pm 1, \ldots, \pm\frac{\nu-1}{2}, \qquad [15]$$

where

$$\nu^3 = N. \qquad [16]$$

Then one has

$$\sum_m e^{-iu|k_m|t} = \frac{\sin\frac{\pi ut}{a}}{\sin\frac{\pi ut}{\nu a}} - i\,\frac{2\sin\frac{\pi ut}{a}\frac{\nu-1}{2\nu}\sin\frac{\pi ut}{a}\frac{\nu+1}{2\nu}}{\sin\frac{\pi ut}{\nu a}}$$

$$\to \nu e^{-i(\pi ut/2a)}\frac{\sin\frac{\pi ut}{2a}}{\frac{\pi ut}{2a}}; \qquad [17]$$

the latter version refers to the large-ν limit. Indeed, it is produced directly as the integral

$$\frac{\nu a}{2\pi}\int_{-\pi/a}^{\pi/a} dk\, e^{-iu|k|t}. \qquad [18]$$

Then, beginning with

$$\langle e^{-i\omega t}\rangle = \frac{1}{N}\sum_\phi e^{-i\omega_\phi t} = e^{-i\underline{\omega}t}\left(\frac{1}{\nu}\sum_m e^{-iu|k_m|t}\right)^3, \qquad [19]$$

the large-ν limit emerges as

$$\langle e^{-i\omega t}\rangle = e^{-i\langle\omega\rangle t}\left(\frac{\sin\frac{\pi ut}{2a}}{\frac{\pi ut}{2a}}\right)^3, \qquad [20]$$

where

$$\langle\omega\rangle = \underline{\omega} + \frac{3\pi u}{2a}. \qquad [21]$$

Examples of the information contained in this complete description of the phonon spectrum are

$$\langle\omega^2\rangle = \langle\omega\rangle^2 + \left(\frac{\pi u}{2a}\right)^2,$$

$$\langle\omega^4\rangle - \langle\omega^2\rangle^2 = 4\left(\frac{\pi u}{2a}\right)^2\left[\langle\omega\rangle^2 + \frac{2}{5}\left(\frac{\pi u}{2a}\right)^2\right]. \qquad [22]$$

The second entry makes explicit the short-time behavior in Eq. **9**.

The long-time characteristics implied by Eq. **8** and the real part of Eq. **20**, for the circumstance $u/a << \langle\omega\rangle$, or $\langle\omega^2\rangle \approx \langle\omega\rangle^2$, are

$$E_\alpha(t)/E \approx \left(\frac{\sin\frac{\pi ut}{2a}}{\frac{\pi ut}{2a}}\right)^6 \to \frac{5}{16}\left(\frac{2a}{\pi ut}\right)^6, \qquad [23]$$

where the latter statement incorporates the average over the time interval $2a/u << t$. More generally, there is a reverberation effect that brings the energy $E_\alpha(t)$ of Eq. **8** down to zero at all $t > 0$ that are an integer multiple of $2a/u$.

For any constituent $a \neq \alpha$, the D-level implications of Eq. **5** are

$$(\mathbf{r} - \mathbf{r}_0)(t)_a = \mathbf{D}(\cos\Omega t)_{a\alpha}$$

and

$$\mathbf{p}(t)_a = M\mathbf{D}\frac{d}{dt}(\cos\Omega t)_{a\alpha}, \qquad [24]$$

where, according to the general form of Eq. **3**,

$$(\cos\Omega t)_{a\alpha} = \langle\cos\omega t e^{i\mathbf{k}\cdot\mathbf{r}_{0a}}\rangle = \mathrm{Re}\,\frac{1}{N}\sum_\phi e^{-i\omega_\phi t}e^{i\mathbf{k}_\phi\cdot\mathbf{r}_{0a}}. \qquad [25]$$

Then, with the introduction of the dispersion relation of Eq. **13**, one has

$$\frac{1}{N}\sum_\phi e^{-i\omega_\phi t}e^{i\mathbf{k}_\phi\cdot\mathbf{r}_{0a}} = e^{-i\underline{\omega}t}\prod_{xyz}\frac{1}{\nu}\sum_m e^{-iu|k_m|t}e^{ik_m\xi}, \qquad [26]$$

where ξ appears as a stand-in for the x, y, or z component of $\mathbf{r}_{0a}$.

The large-ν limit of an individual factor in Eq. **26** is

$$\frac{1}{\nu}\sum_m e^{-iu|k_m|t}e^{ik_m\xi} \to \frac{a}{2\pi}\int_0^{\pi/a} dk\, e^{ik(\xi-ut)} + \frac{a}{2\pi}\int_0^{\pi/a} dk\, e^{-ik(\xi+ut)}$$

$$= \frac{1}{2}\exp\left[i\frac{\pi}{2a}(\xi - ut)\right]\frac{\sin\frac{\pi}{2a}(\xi-ut)}{\frac{\pi}{2a}(\xi-ut)} + \frac{1}{2}\exp\left[-i\frac{\pi}{2a}(\xi+ut)\right]\frac{\sin\frac{\pi}{2a}(\xi+ut)}{\frac{\pi}{2a}(\xi+ut)}. \qquad [27]$$

The two terms represent phonon pulses moving positively and negatively, at the speed u, along the particular axis to which ξ refers. Accordingly, the triple product in Eq. **26** contains $2^3 = 8$ terms that describe phonon pulses moving at the speed $3^{1/2}u$ along the three-dimensional lines that project into the diagonals of the three orthogonal planes that form each octant.

Under the circumstance $ut >> a$, the two pulses of Eq. **27** have no significant overlap and one can focus separately on each of the eight pulses, moving along a straight line that is contained in one of the octants.

The energy associated with a particular constituent, in one of the octants, has the same form as in Eq. **8**, but with $\langle\cos \omega t\rangle$ replaced by the structure of Eq. **25**. If, for simplicity, one again considers a narrow phonon spectrum, $\langle\omega\rangle >> u/a$, the energy associated with a particular lattice site in one of the octants, say the one with all positive coordinates, is given by

$$E_a(t)/E = \frac{1}{8^2}\prod_{xyz}\left[\frac{\sin\frac{\pi}{2a}(\xi - ut)}{\frac{\pi}{2a}(\xi - ut)}\right]^2. \quad \textbf{[28]}$$

One expects that, in the long run, the energy E is distributed through the lattice, with $E/8$ appearing in each octant. Should a pulse center happen to coincide with a lattice site at time t ($\xi - ut = 0$ for x, y, and z), one-eighth of the octant quota would be localized at that site.

More generally, let each $\xi - ut$ be written as the sum of ma, $m = 0, \pm1, \ldots$, and the residue ρ, $|\rho| \le a/2$. Then the expected total energy will be realized if

$$\sum_{m=-\infty}^{\infty}\left[\frac{\sin\frac{\pi}{2a}(ma + \rho)}{\frac{\pi}{2a}(ma + \rho)}\right]^2 = 2. \quad \textbf{[29]}$$

For $\rho = 0$, this assertion reads

$$1 + \frac{8}{\pi^2}\left(1 + \frac{1}{3^2} + \frac{1}{5^2} + \ldots\right) = 2, \quad \textbf{[30]}$$

which is true. Should $\rho = a/2$, one is told that

$$\frac{16}{\pi^2}\left(1 + \frac{1}{3^2} + \frac{1}{5^2} + \ldots\right) = 2, \quad \textbf{[31]}$$

which is also true.

A general mathematical proof—as contrasted with the preceding physical proof—follows from the Fourier series

$$\sum_{m=-\infty}^{\infty} e^{ik(ma+\rho)} = \frac{2\pi}{a}\sum_{\mu=-\infty}^{\infty} e^{i(2\pi\rho/a)\mu}\delta\left(k - \frac{2\pi}{a}\mu\right). \quad \textbf{[32]}$$

Multiplication by $[1 - (k/K)]/K$, with a positive $K < 2\pi/a$, followed by k-integration from $-K$ to K, yields

$$\sum_{m=-\infty}^{\infty}\left[\frac{\sin\frac{1}{2}K(ma + \rho)}{\frac{1}{2}K(ma + \rho)}\right]^2 = \frac{2\pi}{Ka}; \quad \textbf{[33]}$$

the choice $K = \pi/a$ reproduces Eq. **29**.

1. Schwinger, J. (1990) *Proc. Natl. Acad. Sci. USA* **87**, 6983–6984.