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Forced Vibrations of a Harmonic Lattice in Quantum Mechanics*

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Schrödinger's equation is solved in an elementary fashion for a harmonic lattice subject to external forces that are functions explicitly only of time, and to damping forces proportional to velocity expectation values. The result shows that the response is a purely classical motion of the quantum mechanical probability distribution associated with the free lattice. The energy of the lattice is $E_q + E_e$, where E_q is any energy eigenvalue of the free undisturbed lattice existing before the external forces were applied, and E_e is the energy that would be obtained by classical mechanics for the response of the lattice to the disturbance. The energy propagates through the lattice as a purely classical wave motion superposed on any quantum mechanical background that may happen to exist.

Anharmonic coupling terms are needed to cause quantum excitations and produce thermal equilibrium within the lattice. The conventional treatment of energy transport as due to unidirectional normal modes is criticized.

INTRODUCTION

IT is well known that probability wave packets can be formed from solutions of Schrödinger's equation for the simple harmonic oscillator in such a way that the center of the probability distribution oscillates in precisely the same fashion as the classical motion of the oscillator.^{1,2} The same general result has also been proved for forced coupled harmonic oscillators³ when the external force is restricted to being an explicit function only of time.

In this paper we give a simplified discussion of this last problem and point out some surprising implications of the results.

THE FORCED OSCILLATOR SUBJECT TO DAMPING

The Schrödinger equation for this problem is written

$$-\left(\frac{\hbar^2}{2m}\right)\partial^2\psi/\partial q^2 + \frac{1}{2}Kq^2\psi - F(t)q\psi - i\hbar\eta q \int \bar{\psi}(\partial\psi/\partial q')dq'\psi = i\hbar\partial\psi/\partial t. \quad (1)$$

Here, $F(t)$ is the external force, and $i\hbar\eta \int \bar{\psi} \times (\partial\psi/\partial q')dq' = -\eta\langle v \rangle$ is the damping force proportional to the velocity expectation.⁴ To solve

this we change to a variable z :

$$z = q - x(t), \quad (2)$$

and seek the function $x(t)$ such that ψ has the form

$$\psi = U(z) \exp[-iB(q,t)/\hbar], \quad (3)$$

where $U(z)$ is a solution of the Schrödinger equation for a free undamped oscillator:

$$-\left(\frac{\hbar^2}{2m}\right)\partial^2 U(z)/\partial z^2 + \frac{1}{2}Kz^2 U(z) = E_0 U(z). \quad (4)$$

It turns out that (3) satisfies (1) if

$$B(q,t) = E_0 t + \int \left[\frac{1}{2}m\dot{x}^2 - \frac{1}{2}Kx^2 + (Kx - F + m\eta\dot{x})q \right] dt \quad (5)$$

and

$$m\ddot{x} = -Kx + F(t) - m\eta\dot{x}. \quad (6)$$

From Eqs. (2) and (4), the relation $q = x(t)$ locates the center of the quantum mechanical probability packet, and from Eq. (6) this center moves in response to the force $F(t)$ exactly as the classically damped oscillator would. Moreover, the energy expectation of the system is given by

$$\langle E \rangle = i\hbar \int \bar{\psi}(\partial\psi/\partial t) dq = E_0 + \frac{1}{2}m\dot{x}^2 + \frac{1}{2}Kx^2 - Fx + m\eta x\dot{x}, \quad (7)$$

which is exactly the sum of the classical energy and the quantum energy E_0 .

* Supported in part by research funds of Washington State University.

¹ Saul Epstein, *Am. J. Phys.* **27**, 291 (1959).

² I. F. Goldman *et al.*, *Problems in Quantum Mechanics* (Academic Press Inc., New York, 1961), p. 136.

³ M. Kolsrud, *Phys. Rev.* **104**, 1186 (1956).

⁴ Note that the velocity expectation is zero in any eigenstate of the free lattice.

LATTICE OF PARTICLES WITH HARMONIC PAIR INTERACTIONS

Consider N particles each with mass μ and having three degrees of freedom. To make the model as general as possible we can label all the degrees of freedom by a single index, so there are $3N$ coordinates q_m , $m=1,2,\dots,3N$. These coordinates are to be interpreted as displacements from the equilibrium lattice positions. Consider only simple harmonic pair interactions and write the interaction potential as

$$V(q) = \frac{1}{4} \sum_{m,n} K_{mn} (q_m - q_n)^2. \tag{8}$$

Both m and n are here summed over the entire range of values. This form is not restricted to nearest neighbor interaction. Again to maintain maximum generality we shall write the potential giving rise to the external forces in the form

$$W(q,t) = - \sum_m F_m(t) q_m \tag{9}$$

so that $F_m(t)$ is the purely time-dependent force acting on the m th degree of freedom. If the system were a crystal with some boundary, and the external forces were applied only at the boundaries, then all components of $W(q,t)$ would be zero except for those acting on degrees of freedom of the particles in the boundary. We shall also include damping on each degree of freedom proportional to the velocity expectation. Then Schrödinger's equation assumes the form

$$-\left(\hbar^2/2\mu\right) \sum_m (\partial \psi / \partial q_m^2) + V(q)\psi - \sum_m F_m q_m \psi - i\hbar\eta \sum_m q_m \int \bar{\psi} (\partial \psi / \partial q_m') dq_m' \psi = i\hbar \partial \psi / \partial t. \tag{10}$$

The $3N$ variables q_m and the time t are all independent variables in this equation. We now set new variables

$$z_m = q_m - x_m(t) \tag{11}$$

and seek functions $x_m(t)$ of time such that

$$\psi = U(z) \exp(-iB(q,t)/\hbar), \tag{12}$$

with $U(z)$ a solution for the free lattice

$$-\left(\hbar^2/2\mu\right) \sum_m \partial^2 U(z) / \partial z_m^2 + V(z) U(z) = E_0 U(z), \tag{13}$$

where

$$V(z) = \frac{1}{4} \sum_{m,n} K_{mn} (z_m - z_n)^2. \tag{14}$$

It turns out that (12) satisfies (10) if

$$B(q,t) = E_0 t + \int \left[\frac{1}{2} \mu \sum_m \dot{x}_m^2 - \frac{1}{2} \sum_{m,n} K_{mn} (x_m - x_n)^2 + \frac{1}{2} \sum_{m,n} K_{mn} (x_m - x_n) (q_m - q_n) - \sum_m F_m q_m + \mu\eta \sum_m \dot{x}_m q_m \right] dt \tag{15}$$

and the functions $x_m(t)$ satisfy the equations

$$\mu \ddot{x}_m = - \sum_n K_{mn} (x_m - x_n) + F_m - \mu\eta \dot{x}_m. \tag{16}$$

These are exactly the classical equations of motion of the lattice in response to the external forces and damping terms. Therefore, the centers at $q_m = x_m(t)$ of the quantum packets follow the classical motion of the lattice. Again the energy expectation of the lattice is a simple sum of the quantum excitation E_0 and the energy of the classical motion

$$\langle E \rangle = E_0 + \frac{1}{2} \mu \sum_m \dot{x}_m^2 + \frac{1}{4} \sum_{m,n} K_{mn} (x_m - x_n)^2 - \sum_m F_m x_m + \mu\eta \sum_m x_m \dot{x}_m. \tag{17}$$

TRANSPORT PHENOMENA IN A HARMONIC LATTICE

If the general results of this paper are applied for instance to a linear chain lattice of coupled oscillators, driven with a force at one end and appropriately loaded with force at the other end, it becomes apparent that we have a description of *classical* energy propagation through the lattice as an exact solution to the Schrödinger equation.

In the conventional quantum theory of propagated waves in an ideal lattice,⁵ the normal modes are resolved into oppositely propagating components, and the component propagating in the direction of interest is accepted as repre-

⁵ J. M. Ziman, *Electrons and Phonons* (Oxford University Press, New York, 1960).

senting the transport of energy. The question of how this energy is supplied at one boundary and removed at the other is avoided by adopting cyclic boundary conditions. This in effect means that the crystal bends back on itself, and there is no boundary at which the energy is supplied. We are therefore discussing an internal current whose origin in history is obscure; yet it is this current whose future history is studied in the usual theory of resistance by means of the quantum theory of scattering. It is of course openly admitted⁶ that the cyclic crystal is a physical impossibility; one would have to bend the crystal back on itself in all three dimensions to do what the theory requires. But boundary errors are excused by the remark that if we make the crystal large enough, we push the boundaries off to infinity and can then hope that the errors go down as the ratio of surface to volume. While such a procedure is a familiar device, the thesis of this paper is that it has trapped us into a quite serious error in the present instance.

When one examines the problem classically, the appropriate boundary conditions for an isolated lattice induce a discrete normal mode spectrum exactly as in quantum theory; but the spectrum of propagated waves, driven by arbitrary forces at the boundary, is not discrete and indeed has no relation with the spectrum of normal modes. Obviously forced vibrations must have the same spectral structure as the driving force, and the continuity of this spectrum is not a result of having a large crystal. The same result is also true of the correct quantum theory: The propagated wave is not derived from the standing wave analysis, but is superposed on them.

This result will have important consequences for the theory of electrical resistance; rather than, as in the past, discussing electron-phonon interactions, we should discuss the coupling between electrons and the classical waves modulating the lattice states. Because the spectrum of these classical waves is essentially continuous and determined by the boundary fluctuations on the lattice, and not determined by the normal modes of the isolated lattice, there may be significant differences compared with the theories currently in use. These theories have

⁶ Reference 5, p. 19.

certainly been eminently successful in correlating experimental results, and we are not suggesting that they be abandoned for purely logical reasons. A logically questionable theory that works in practice is better than a logically perfect theory that makes no predictions that can be tested. But the point is that a student should be aware of the logical weaknesses of the successful theory, and so be alert for possible future improvements.

EXCITATION OF THE HARMONIC LATTICE

For ease of visualization, consider again a linear chain of oscillators each coupled only to its two neighbors, and let external forces $F(t)$ and $G(t)$ act on the two ends of the chain.

Suppose the chain to be set up initially in one of the quantum standing modes, with the forces $F(t)$ and $G(t)$ initially zero. Then beginning at some time t_0 let a pulse $F(t)$ of some arbitrary form be applied at one end. The response of the chain to this is, according to the exact solution of the Schrödinger equation, a classical pulse propagating down the chain, modulating the quantum mechanical wave function as it propagates. Then as this pulse arrives at the other end of the chain, let a load $G(t)$ be applied, matched exactly with the arriving pulse, in such a way that the energy is completely absorbed as it emerges. The final result is that the chain returns exactly to its original quantum state. There is no mechanism here by which the classical energy pulse can be transferred during propagation into a quantum of excitation of the chain in such a way that, on removing the energy pulse emerging at the end, the chain is left in a quantum state different from its initial state.⁷

It is of course true that, while the classical energy is present in the lattice, the quantum state can be expressed as a linear superposition of

⁷ The analogous theorem for a simple harmonic oscillator is implied by results given in reference 2, problem 3.17. In fact it is proved there that the transition probability from any initial simple harmonic eigenstate to any other such eigenstate, due to an arbitrary time-dependent perturbing force, depends on the total (classical) work w done by the force during its action. It turns out that if w is zero, all the transition probabilities vanish, and the final state is identical with the initial state. The system can thus be taken through a variety of superposition states and returned to its initial eigenstate simply by arranging for the perturbing force to return the classical energy to its initial zero value.

the entire spectrum of its free-vibration quantum states. However, we venture to make the somewhat heretical statement that this is a mathematical theorem with no very real physical significance. The formal physical significance is of course contained in the familiar remark that the square amplitude of any component in such a superposition is the probability that the lattice would be found to have the energy of the corresponding quantum state if a suitable series of measurements were to be made on the lattice. Now it might be a rewarding experience to attempt to devise a "gedanken" apparatus that could be tuned to respond to the lattice with a "yes" or "no" signal according to whether the lattice was or was not in any selected quantum state of any of its modes of free vibration. Such an apparatus would then display the probability distribution of the propagating wave packet. But, in practice, it would seem that the best we can do in fact is to measure the energy fed into the lattice at one end and drawn out at the other. And according to the exact solution we have been discussing, this energy is necessarily classical, has a classically continuous spectrum, and is completely independent of the quantum mechanical background that may be present in the lattice. Any observation of the lattice by means of time-dependent loads—one might call them sensing devices—will reveal only the classical modulation, and will not either reveal or change the quantum mechanical background.

This result may have important consequences for the theory of thermal equilibrium in crystals.

If we neglect radiation effects, any real crystal

placed in a thermal bath maintains its thermodynamic equilibrium through a mechanism of fluctuating pressures over its surfaces. In an ideal crystal these fluctuations can have only classical effects on the motion of the lattice, which are superposed on the quantum states without influencing the energy of the latter.

In a real crystal a coupling mechanism must exist which permits an exchange of energy between classical propagating waves and the quantum mechanical steady states. The same coupling mechanism will be responsible for the transitions between states needed to adjust the energy distribution in the crystal to the temperature of the bath. A complete theory of this anharmonic coupling mechanism must be discovered before we can claim to understand the thermodynamical equilibrium of crystal lattices.

It is worthwhile to think of the analogy between the collection of normal modes of an ideal harmonic lattice, and the particles of an ideal gas. There is no coupling between the normal modes, and there are no collisions in an ideal gas. There can be no transitions between the quantum states of the ideal lattice, and neither can an ideal gas change its state. The collisions in a real gas involve interactions and the gas is nonideal; a coupling between normal modes can exist only through anharmonic terms, and the lattice is no longer ideal. Any small fluctuation on the walls containing an ideal gas can only send a few atoms charging clear across to the other side without modifying the rest of the gas; collisions, or anharmonic terms, are essential for the attainment of thermodynamic equilibrium.