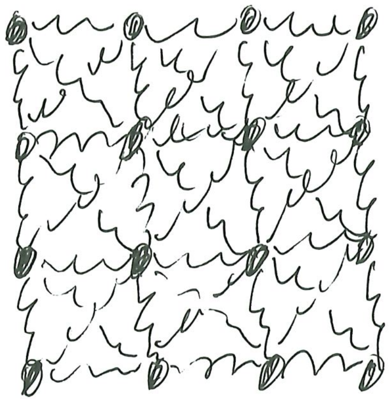
F. Each normal mode is an independent harmonic oscillator



Real situation
Many atoms with coupled Motions (Complicated!)

$\omega(\vec{q})$
↑
Normal mode frequencies

System is equivalent to

$$H = \sum_n \frac{p_n^2}{2m} + \frac{K}{2}\sum_n (u_n - u_{n+1})^2$$

(coupled oscillators)

↓ transform into

$$\sum_{\vec{q}} (\text{oscillator of } \omega(\vec{q}))$$

Example : Monatomic Chain

Coupled eqs. of motion $M\ddot{u}_n = K(u_{n+1} + u_{n-1} - 2u_n)$ (1)

and $\omega(q) = \sqrt{\frac{4K}{M}}\left|\sin\left(\frac{qa}{2}\right)\right|$ are normal mode frequencies (3)

General form of

$$\boxed{\underset{\text{real}}{u_n(t)} = \sum_q \left(e^{iqna} \underbrace{e^{-i\omega(q)t} \frac{A_q}{\sqrt{N}}}_{\text{to become } B_q(t)} + e^{-iqna} \underbrace{e^{i\omega(q)t} \frac{A_q^*}{\sqrt{N}}}_{\text{to become } B_q^*(t)} \right)} \quad (13)$$

Euler Equation: $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{u}_n}\right) - \frac{\partial L}{\partial u_n} = 0$ (14) L = Lagrangian

What is the proper $L(u_n, \dot{u}_n)$ that gives correct eq. of motion (Eq.(11))?

coordinates velocities [c.f. $L(q, \dot{q})$]

$$L = \sum_{n=1}^{N} \frac{1}{2} M \dot{u}_n^2 - \frac{1}{2} \sum_{n=1}^{N} K (u_n - u_{n+1})^2 \quad \text{works} \quad (15)$$

It follows that $p_n = \frac{\partial L}{\partial \dot{u}_n}$ is conjugate momentum to coordinate u_n, i.e. $p_n = M\dot{u}_n$ (16)

H = Hamiltonian = $\sum_n p_n \dot{u}_n - L$ (Legendre Transform from L to H)

(classical mechanics)

$$= \sum_n \frac{p_n^2}{2M} + \frac{K}{2} \sum_n (u_n - u_{n+1})^2 \quad (16)$$

(would have guessed)

Comments

- Eq. (13) is a key step in understanding what "phonons" are!
  (and what "photons" are, and in every quantization of fields†)
- It is expanding the displacements in the normal mode oscillations
- The coefficients A_q, A_q^* will play important roles when we quantize the system
- $u_n(t)$ are the derivations from perfect periodicity

  electron sees $U_{\text{periodic}}(\vec{r}) = \sum_n U_{\text{atom}}(\vec{r}-\vec{R}_n) \Rightarrow$ bands

  But when electron sees $\sum_n U_{\text{atom}}(\vec{r}-(\vec{R}_n+u_n(t))) \approx U_{\text{periodic}}(\vec{r}) + \overbrace{\text{Extra terms}}^{\text{leading term} \sim u_n(t)}$

  Quantum theory: $\psi_{n\vec{k}}(\vec{r}) \xrightarrow[\text{electron-phonon interaction}]{} \psi_{n'\vec{k}'}(\vec{r})$

---

† We don't have fields yet. The $u_n(t)$'s are for discretized n (the atom at n^{th} cell). For a string ($q \to 0$ limit), we can consider the displacement field $u(x,t)$ of the bit of string at x and time t, then we have a field.

$$H = \sum_n \frac{p_n^2}{2M} + \frac{K}{2} \sum_n (u_n - u_{n+1})^2$$

for $p_n = M\dot{u}_n$ use Eq. (13)

use Eq. (13) to write p_n

(after a few pages of equations)

$$H = \sum_q M\,\omega^2(q) \left[B_q^*(t)\, B_q(t) + B_q(t)\, B_q^*(t) \right] \qquad (17)$$

$$H = \sum_q M\omega^2(q)\left[B_q^*(t)\,B_q(t) + B_q(t)\,B_q^*(t)\right] \quad (17)$$

- still 100% classical mechanics
- intentionally written in a form for imposing QM rule

$$= \sum_q \frac{\hbar\omega(q)}{2}\left[b_q^*(t)\,b_q(t) + b_q(t)\,b_q^*(t)\right] \quad (18)$$

where $B_q(t) \equiv \sqrt{\dfrac{\hbar}{2M\omega(q)}}\; b_q(t)$

- still classical mechanics
- "$\hbar$" cancels out

What for?

- Must know (identify) coordinate-momentum pairs before imposing QM rule

Now, quantize the problem (this is formally "first quantization")

$$\underset{\text{coordinates}}{u_n} \rightarrow \underset{\text{operators}}{\hat{u}_n} \;;\; \underset{\text{momenta}}{p_n} \rightarrow \underset{\text{operators}}{\hat{p}_n} \;;\; \underbrace{[\hat{p}_n, \hat{u}_{n'}] = -i\hbar\,\delta_{nn'} \;;\; [\hat{u}_n, \hat{u}_{n'}] = 0,\; [\hat{p}_n, \hat{p}_{n'}] = 0}_{\text{impose QM commutators}} \quad (19)$$

[It is at this step that we "quantize" the coupled oscillators problem.]

Recall $u_n(t) = \sum_q \left(B_q(t)\, e^{iqna} + B_q^*(t)\, e^{-iqna} \right)$ $\quad \therefore\ u_n(\{B_q(t), B_q^*(t)\})$

$p_n = M\dot{u}_n \Rightarrow p_n(\{B_q, B_q^*\}) \rightarrow B_q(u_n, p_n)\ ;\ B_q^*(u_n, p_n)$ †

As $u_n \rightarrow \hat{u}_n$, $p_n \rightarrow \hat{p}_n$; $B_q \rightarrow \hat{B}_q$; $B_q^* \rightarrow \hat{B}_q^*$

$[\hat{u}_n, \hat{p}_{n'}] = i\hbar\, \delta_{nn'} \Rightarrow [\hat{B}_q, \hat{B}_{q'}^*] = \dfrac{\hbar}{2M\omega(q)}\, \delta_{qq'}$ (20)

OR $[\hat{b}_q, \hat{b}_{q'}^+] = \delta_{qq'}$ (21) $\left(\hat{b}_q \equiv \sqrt{\dfrac{2M\omega(q)}{\hbar}}\, \hat{B}_q \right)$

After imposing QM: $H \rightarrow \hat{H}$

$$\hat{H} = \sum_q \underbrace{\left(\frac{\hbar\omega(q)}{2} + \hbar\omega(q)\, \hat{b}_q^+ \hat{b}_q \right)}_{\text{Harmonic oscillator QM Hamiltonian of angular freq. } \omega(q)} \qquad (22)$$

Quantum Mechanical!

sum over normal modes labelled by q

---

† For those with the experience of handling $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}K\hat{x}^2$, this step is analogous to defining $\hat{a}$ and $\hat{a}^+$ by combining $\hat{x}$ and $\hat{p}$, e.g. $\sim(\hat{x} + i\hat{p})$, $(\hat{x} - i\hat{p})$ with some factors ignored.

For each oscillator labelled by q (or $\omega(q)$):

allowed energies are $\underbrace{\frac{1}{2}\hbar\omega(q)}_{\text{ground state (zero point) energy}} + n_\omega \hbar\omega(q)$ with $n_\omega = 0, 1, 2, 3, \cdots$

n_ω: labels excitation of oscillator

<u>Phonons of the mode $\omega(q)$:</u>

$n_\omega = 0$, no phonon

$n_\omega = 1$, 1 phonon (energy $\hbar\omega(q)$, momentum $\hbar q$ (see Eq. (13))

$n_\omega = 2$, 2 phonons (each $\hbar\omega(q)$ energy, each $\hbar q$ momentum)

$\vdots$

This is the real meaning of phonons being quantas of lattice vibrations!

[Same idea goes to all other q's (and all branches)]

Formally, the state of the phonon description is given by

$$|n_{q_1}, n_{q_2}, n_{q_3}, \cdots \rangle \quad (23)$$

[a "q" gives a $\omega(q)$, for one branch]

Generally,

$$|\{n_{s,\vec{q}}\}\rangle \quad (23a)$$

s labels branch; $\vec{q} \in$ B.Z.

The corresponding energy (follows from Eq. (22))

$$= \sum_{q} \left(n_q + \frac{1}{2}\right)\hbar\omega(q) \quad (24)$$

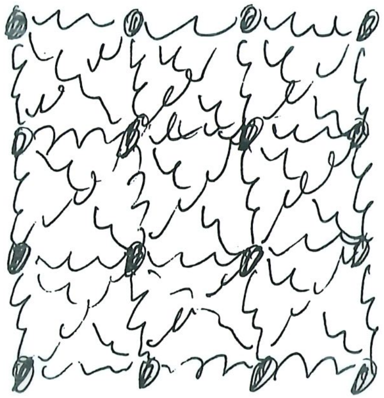
n_q gives # phonons of a particular normal mode

Corresponding energy

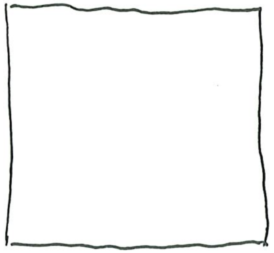
$$= \sum_{s}\sum_{\vec{q}} \left(n_{s,\vec{q}} + \frac{1}{2}\right)\hbar\omega_s(\vec{q}) \quad (24a)$$

higher dimensions, several atoms per unit cell

A profound idea



Actual System



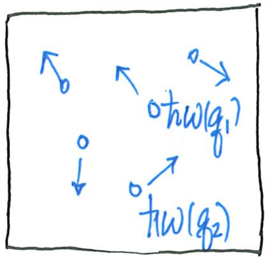
$T=0$

[no phonons of all modes] ("Nothing"!)

(simple picture)

AND "Nothing" (vacuum is something)

$\left(\sum_q \frac{1}{2}\hbar\omega_q \right)$

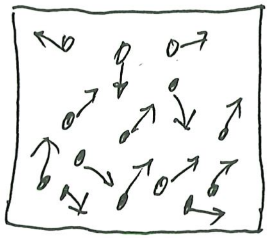


Low Temp

some phonons excited

"Collective Excitations"

$\underbrace{\text{Collective}}_{\text{all atoms are involved}}$



High Temp

more phonons excited

Picture: Electrons see deviations from perfect periodicity $\Rightarrow$ electrons see phonons [electron-phonon scattering leads to resistance]

Phonon-phonon (anharmonic term) interactions lead to thermal conduction.

G. More physics to learn: What QFT is about?

- From chain to string ("easier"!) [always long wavelength limit]

$$\rho \frac{\partial^2 u(x,t)}{\partial t^2} - C \frac{\partial^2 u(x,t)}{\partial x^2} = 0 \quad (25)$$ [Wave Equation $\Leftrightarrow$ equations of motion]

$u(x,t)$ = displacement field (from equilibrium)

Try $e^{iqx-i\omega t}$?

normal modes

$$\omega^2(q) = \frac{C}{\rho} q^2 \quad \text{OR} \quad \omega = \sqrt{\frac{C}{\rho}}\, q \quad (26)$$ [phonon dispersion relation]

no atomic periodicity (don't need B.Z.'s)

(only acoustic $q \to 0$ behavior)

$$L = \int_0^L \left[\frac{1}{2}\rho\left(\frac{\partial u(x,t)}{\partial t}\right)^2 - \frac{1}{2}C\left(\frac{\partial u(x,t)}{\partial x}\right)^2\right] dx$$

$$\equiv \int_0^L \underbrace{\mathcal{L}}_{\text{"Lagrangian density"}}\, dx = \text{Lagrangian works with}$$

c.f. $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} = 0$ (discrete)

$$\frac{\partial \mathcal{L}}{\partial u(x,t)} - \frac{\partial}{\partial x}\left(\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial u}{\partial x}\right)}\right) - \frac{\partial}{\partial t}\,\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial u}{\partial t}\right)} = 0$$ is the Euler-Lagrange Equation for continuum system

Conjugate momentum $\Pi(x)$ to $u(x)$ is $\rho\dot{u}(x)$ [defined by $\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial u}{\partial t}\right)}$]

conjugate pair!

$$H = \text{Hamiltonian} = \int \dot{u}(x)\,\Pi(x)\,dx - L = \int_0^L \left[\frac{\Pi(x)^2}{2\rho} + \frac{C}{2}\left(\frac{\partial u}{\partial x}\right)^2\right] dx \equiv \int \mathcal{H}\,dx$$

Hamiltonian Density

This is classical field Theory.

Q: What if we start the exercise with Maxwell's Wave Equation for EM waves?

- a bit more complicated (vector fields)
- but same idea

To prepare for quantizing the classical displacement field, do the same expansion using normal modes $e^{iqx-i\omega t}$ $(\omega \sim q)$

coordinates

$$u(x,t) = \sum_q \Big(\underbrace{B_q(t)}\, \overbrace{\frac{1}{\sqrt{L}} e^{iqx}}^{\text{normal modes}} + \underbrace{B_q^*(t)}\, \frac{1}{\sqrt{L}} e^{-iqx} \Big) \quad ; \quad \pi(x,t) = \rho\, \dot{u}(x,t)$$

coefficients to become operators upon quantization

$$= \sum_q \frac{1}{\sqrt{L}} \sqrt{\frac{\hbar}{2\rho\omega(q)}} \left(b_q e^{iqx} + b_q^* e^{-iqx} \right) \quad (27) \qquad \left(b_q \equiv \sqrt{\frac{2\rho\,\omega(q)}{\hbar}}\, B_q \right)$$

conjugate momentum

$$\pi(x,t) = \rho\, \dot{u}(x,t) = \sum_q \frac{i}{\sqrt{L}} \sqrt{\frac{\hbar\omega(q)\rho}{2}} \left(-b_q e^{iqx} + b_q^* e^{-iqx} \right) \quad (28)$$

still classical theory

Quantization of the displacement field

$\hat{u}(x,t)$, $\hat{\pi}(x,t)$ "field operators" (then $b_q \to \hat{b}_q$; $b_q^* \to \hat{b}_q^+$)

$$\boxed{\begin{aligned} [\hat{\pi}(x,t), \hat{u}(x',t')] &= \frac{\hbar}{i}\delta(x-x')\delta(t-t') \\ [\hat{\pi}(x,t), \hat{\pi}(x',t')] = 0 &= [\hat{u}(x,t), \hat{u}(x',t')] \end{aligned}} \quad (29)$$

c.f. $[\hat{p}, \hat{x}] = \frac{\hbar}{i}$ (only one pair)

$[\hat{p}_i, \hat{x}_j] = \frac{\hbar}{i}\delta_{ij}$ (more pairs)

Impose these rules, then H becomes

$$H = \sum_q \hbar\omega(q)\left(b_q^+ b_q + \frac{1}{2}\right) \quad (30)$$

with $[\hat{b}_q, \hat{b}_{q'}^+] = \delta_{qq'}$, $[\hat{b}_q, \hat{b}_{q'}] = 0 = [\hat{b}_q^+, \hat{b}_{q'}^+]$

(oscillators again!)

The displacement field has been quantized

"Quantum Field Theory"

Q: Repeat exercise for Maxwell's Wave Equation

$\Rightarrow$ Quantization of EM fields

$$H = \sum_q \hbar\omega(q)\left(a_q^+ a_q + \frac{1}{2}\right)$$

photons! (also oscillator physics)

Remarks

- How about taking an already quantum mechanical equation and pretending it to be a wave equation, and carrying out the process again?

e.g

(i) $$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) \ ?$$ (Schrödinger)

(ii) $$\frac{1}{c^2}\frac{\partial^2 \Psi(x,t)}{\partial t^2} - \nabla^2 \Psi(x,t) + \frac{m^2c^2}{\hbar^2}\Psi(x,t) = 0 \ ?$$ (Klein-Gordon)

(iii) $$i\hbar \gamma^\mu \partial_\mu \Psi - mc\Psi = 0 \ ?$$ (Dirac)

All can be done! (i) is useful in Condensed Matter Physics. (ii), (iii) and Maxwell eqs. are starting point of QED and standard model [no interactions yet, "free fields"]

In quantizing the fields, you are quantizing an already quantum mechanical equation

$\Rightarrow$ "Second Quantization"

Refs.

- For condensed matter physics using field theoretical methods, see

Altland and Simons, "Condensed Matter Field Theory"

Mahan, "Many-Particle Physics" (using Green's function approach)

Shankar, "Quantum Field Theory and Condensed Matter" (using path integral approach)

- For particle physics, see

Mandl and Shaw, "Quantum Field Theory"

Gross, "Relativistic Quantum Mechanics and Field Theory"