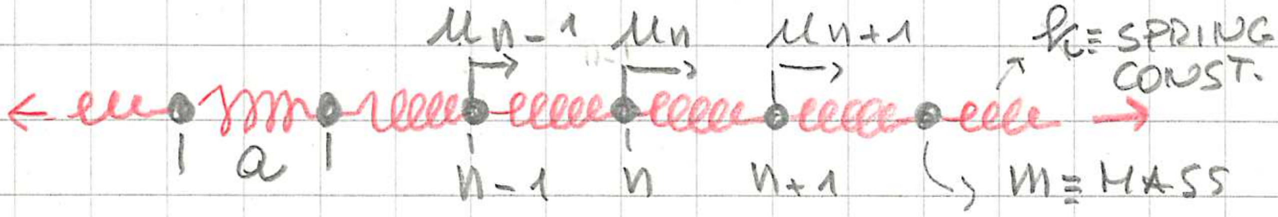
QUANTIZATION OF A 1D VIBRATING LATTICE

THE CLASSICAL HAMILTONIAN OF THE MECHANICAL MASS-SPRING CHAIN OF N MASSES AND N SPRINGS



IS GIVEN BY

$$H = \sum_{n=1}^{N} \left[\frac{p_n^2}{2m} + \frac{k}{2}\left(u_{n+1} - u_n\right)^2 \right]$$

KINETIC POTENTIAL

CLASSICALLY FOR A GIVEN k IT VIBRATES WITH A SINGLE FEQUENCY $\Omega(k)$.
THE ENERGY (AND HENCE THE AMPLITUDE) CAN BE CONTINUUOUSLY VARIED.
THE QUANTIZATION OF THIS HAMILTONIAN CAN BE OBTAINED FOLLOWING THE SAME PROCEDURE WE USED FOR THE QUANTIZATION OF THE E.M. FIELDS. HENCE WE OBTAIN

$$\hat{H} = \sum_{K=1}^{N} \left(\frac{1}{2m} \hat{p}_K^{\dagger} \hat{p}_K + \frac{m\Omega^2}{2} u_K^{\dagger} u_K \right)$$

WHERE $K = m\left(\frac{2\pi}{L}\right)$, $L = Na$ BEING m AN INTEGER AND N THE NUMBER OF THE INDEPENDENT OSCILLATORS.

AT THE SAME TIME WE CAN DEFINE A CREATION AND A ANNIHILATION OPERATORS $\hat{a}^+_k$, $\hat{a}_k$ RESPECTIVELY DEFINED AS

$$\hat{a}^+ = \frac{1}{\sqrt{2\hbar}}\left(\sqrt{m\omega_k}\,\hat{u}_k - \frac{i}{\sqrt{m\omega_k}}\hat{p}_k\right)$$

$$\hat{a} = \frac{1}{\sqrt{2\hbar}}\left(\sqrt{m\omega_k}\,\hat{u}_k + \frac{i}{\sqrt{m\omega_k}}\hat{p}_k\right)$$

$\Rightarrow$

$$\hat{H} = \sum_k{}' \left(a^+_k a_k + \frac{1}{2}\right)\hbar\Omega_k$$ WITH EIGENSTATES

$|n_1, n_2, n_3, \dots\rangle$ $\Rightarrow$

$$\hat{H}|n_1, n_2, n_3, \dots\rangle = \sum_k{}' \left(\hat{n}_k + \frac{1}{2}\right)\hbar\Omega_k |n_1, n_2, n_3, \dots\rangle$$

WHERE $\hat{n}_k$ IS THE NUMBER OPERATOR.

- THE QUANTUM OF ENERGY $\hbar\Omega_k$ IS A COLLECTIVE EXCITATION PARTICLE CALLED PHONON OF THE K-MODE. FOR THIS MODE THERE ARE n_k PHONONS.

- OBSERVATION

AMONG PHONONS THERE ARE NO INTERACTIONS, THEREFORE THEY CONSTITUTE A "FREE PHONON GAS".

IF THERE ARE Z ATOMS IN A UNIT CELL (Z-BRANCHES) THAN THE TOTAL VIBRATIONAL ENERGY OF THE LATTICE IS

$$\hat{H} \equiv U = \sum_{K} \sum_{S=1}^{3} \left(n_{KS} + \frac{1}{2} \right) \hbar \Omega_{K,S}$$

$\sum_{K}$ → MODES

$\sum_{S=1}^{3}$ → PHONON BRANCHES

$\Omega_{K,S}$ → FREQUENCY OF THE MODE K AND BRANCHE S

- OBSERVATION: A PHONON IS A COLLECTIVE EXCITATION IN A PERIODIC ELASTIC ARRANGEMENT OF ATOMS OR MOLECULES IN CONDENSED MATTER, SPECIFICALLY IN SOLIDS AND SOME LIQUIDS. OFTEN PHONONS ARE REFFERED AS "QUASIPARTICLE", A TERM INTRODUCED BY LANDAU. THEY CAN BE VIEWED AS COLLECTIVE EXCITED STATES OF THE VIBRATION MODES OF ELASTIC SYSTEMS.

  IN THE QUANTUM FIELD FORMALISM PHONONS ARE BOSON THEREFORE A BOSON GAS OBEIES TO THE BOSE-EINSTEIN STATISTICS. IN OTHER WORDS A THERMAL EQUILIBRIUM AND IN A HARMONIC REGIME THE PROBABILITY OF FINDING PHONONS IN A GIVEN STATE FOR A GIVEN MODE $(\Omega_{K,S})$ IS

$$\langle n(\Omega_{K,S}) \rangle = \frac{1}{e^{\left(\frac{\hbar \Omega_{K,S}}{K_B T}\right)} - 1}$$

THE WAY WE HAVE OBTAIN THE $\hat{H}$ FOR THE E.M. FIELD AND FOR THE LATTICE VIBRATION IS KNOWN AS SECOND QUANTIZATION OR OCCUPATION NUMBER FORMALISM, WHERE $\hat{n}_k = \hat{a}^+_k \hat{a}_k$ IS THE OCCUPATION NUMBER OF THE K-MODE. THAT IS THE NUMBER OF "QUANTUM OF ENERGY" (PHOTON OR PHONON) THAT OCCUPIES THE MODE. $\hat{n}_k$ IS A HERMITIAN OPERATOR, IMPLING THAT $\hat{n}_k$ IS A PHYSICAL OBSERVABLE. THE LATTICE VIBRATIONS AS DESCRIBED BY THE SECOND QUANTIZATION SHOW THREE IMPORTANT PROPERTIES:

1- PHONONS ARE BOSONS SINCE ANY NUMBER OF IDENTICAL PARTICLES CAN BE CREATED OR DISTROIED BY THE APPLICATION OF THE OPERATOR $\hat{a}^+$ AND $\hat{a}$.

2- EACH PHONON IS A "COLLECTIVE MODE" CAUSED BY THE MOTION OF EVERY ATOM IN THE LATTICE. THIS MAY BE SEEN FROM THE FACT THAT THE $\hat{a}^+$, $\hat{a}$ OPERATORS, DEFINED IN THE MOMENTUM SPACE, CONTAIN SUMS OVER THE POSITION AND MOMENTUM OPERATORS OF EVERY ATOM WHEN WRITTEN IN THE POSITION SPACE (MOMENTUM SPACE $\equiv \mathbb{R}^{-1}$, POSITION SPACE, $\mathbb{R}$)

3- USING THE POSITION-POSITION CORRELATION FUNCTION IT CAN BE SHOWN THAT PHONONS ACT AS WAVE OF THE LATTICE DISPLACEMENT,

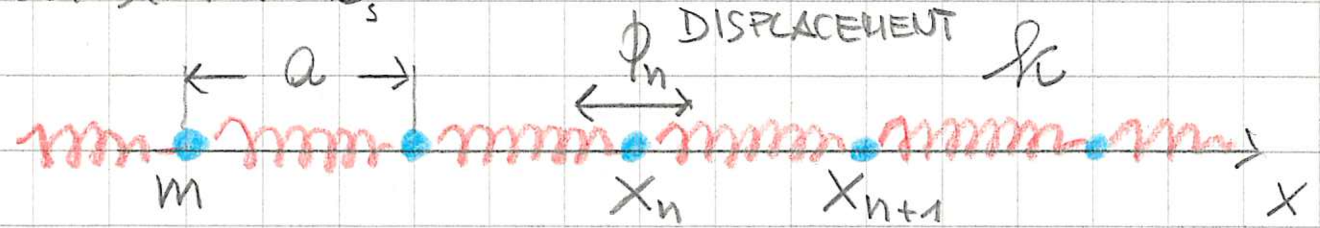
- ACUSTIC PHONONS ARE COHERENT DISPLACEMENTS OF ATOMS OF THE LATTICE OUT OF THEIR EQUILIBRIUM POSITIONS. IF THE DISPLACEMENT IS IN THE DIRECTION OF PROPAGATION OF THE WAVE THAN THE IN SOME REGIONS THE ATOMS WILL BE CLOSER THAN ATOMS AT EQUILIBRIUM AND OTHERS FARTHER APART AS IN SOUND WAVE IN AIR. LONGITUDINAL AND TRANSVERSAL ACOUSTIC PHONONS ARE OFTEN ABBREVIETED AS LA, LT RESPECTIVELY.
- OPTICAL PHONONS ARE OUT-OF-PHASE MOVEMENTS OF ATOMS IN THE LATTICE (ONE ATOM MOVING TO THE LEFT AND ITS NEIGBOR TO THE RIGHT). THEY ARE CALLED OPTICAL BECAUSE IN POLAR CRISTALS FLUCTUATION IN THE DISPLACEMENT CREATE AN ELECTRICAL POLARIZATION THAT COUPLES TO THE E.M. FIELD, HENCE THEY CAN BE EXCITED BY E.M. RADIATION (IR). THE ELECTRIC FIELD OF THE LIGHT WILL MOVE THE POSITIVELY CHARGED IONS IN THE DIRECTION OF THE FIELD AND THE NEGATIVELY CHARGED IONS IN THE OPPOSITE DIRECTIONS CAUSING THE CRYSTAL TO VIBRATE. OPTICAL PHONON HAVE NON-ZERO FREQUENCY AT THE CENTER OF THE BRILLOUIN ZONE (Γ-POINT) WHILE THEY SHOW NO-DISPERSION AT THE BOARDER ZONE $(\pm \pi/a)$ THIS IS BECAUSE THEY CORRESPOND TO A MODE

OF VIBRATION WHERE POSITIVE AND NEGATIVE CHARGED IONS AT ADIACENT LATTICE SITES SWING AGAINST EACH-OTHER CREATING A TIME-VARING DIPOLE MOMENT. THIS PHONONS HAVE A LINEAR INTERACTION WITH LIGHT (IR) AND THEY ARE CALLED INFRARED ACTIVE PHONON. HOWEVER, NOT ALL THE OPTICAL PHONON CAN INTERACT WITH LIGHT BECAUSE OF THE OPTICAL DIPOLE SELECTION RULES, NONETHELESS THIS OPTICAL PHONONS CAN BE DETECTED BY NON-LINER OPTICAL PROCESSES SUCH AS THE RAMAN SCATTERING.
CONVERSELY THE ACOUSTIC PHONONS CAN ONLY BE OPTICALLY DETECTED BY NON-LINEAR OPTICAL SCATTERING KNOWN AS BRILLOUIN SCATTERING.

- A GLANCE TO THE QUANTUM FIELD THEORY OF PHONONS

IN THE FOLLOWING WE WILL DEVELOP A MORE ADVANCED FORMALISEM TO DESCRIBE ON A Q.M. BASE THE LATTICE VIBRATION USING THE LAGRANGE-HAMILTON QUANTUM OPERATORS AS WE HAVE LEARNED FOR THE E.M. FIELDS. THE INTENT IS TO POSE THE BASE FOR DEVELOPING A QUANTUM FIELD THEORY. AS DONE BEFORE WE START WITH A SEMPLIFIED 1-D MODEL CRYSTAL CONSIDERING A CHAIN OF MASSES ALL IDENTICAL WITH MASS m

(ATOMS) CONNECTED BY IDENTICAL SPRINGS OF CONSTANT k_s



LET'S START WITH THE CLASSICAL LAGRANGIAN AND HAMILTONIAN FORMULATION, ASSUMING THAT THE CHAIN IS MADE OF N-ATOMS WITH PERIODIC BOUDERY CONDITIONS $x_{n+1} = nQ + x_1$ WITH $n = 1, 2, \ldots N$.

THE LAGRANGIAN IS GIVEN BY

$$L = T - V = \sum_{n=1}^{N} \left[\frac{m}{2} \dot{x}_m^2 - \frac{k}{2} \left(x_{n+1} - x_n - a \right)^2 \right]$$

IN REAL SOLIDS THE INTERATOMIC POTENTIAL IS MORE COMPLEX BUT AT LOW ENERGY THE HARMONIC CONTRIBUTION DOMINATES.
TAKING THE EQUILIBRIUM POSTION $\bar{x}_n = na$ IT IS ASSUMED THAT THE POSITION DUE TO A SMALL PERTURBATION WILL GIVE A DISPLACEMENT $|x_n(t) - \bar{x}_n| \ll a$ WITH $x_n(t) = \underbrace{\bar{x}_n}_{\text{EQUIL.}} + \underbrace{\phi_n(t)}_{\text{DISPLA.}}$

$$\Rightarrow L = \sum_{n=1}^{N} \left[\frac{m}{2} \dot{\phi}_n^2 - \frac{k}{2} \left(\phi_{n+1} - \phi_n \right)^2 \right]$$

SINCE WE ASSUME ALL THE DISPLACEMENT IDENTICAL $\phi_{N+1} = \phi_1$.

TO OBTAIN CLASSICAL EQ OF MOTION FROM L WE CAN MAKE USE OF THE LEAST ACTION PRINCIPLE THAT WE REMEMBER FOR A SINGLE PARTICLE WITH COORDINATE $x(t)$ REDUCES TO THE EULER-LAGRANGE EQUATION

$$S(x) = \int L(\dot{x}, x)\, dt \rightarrow \frac{d}{dt}(\partial_{\dot{x}} L) - \partial_x L = 0$$

FOR A FREE PARTICLE IN A HARMONIC OSCILLATOR $V(x) = \frac{1}{2} k x^2$

$$L(\dot{x}, x) = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} m \omega^2 x^2$$

HENCE USING THE E-L EQUATION WE OBTAIN

$$m\ddot{x} = -kx$$

MINIMIZING THE CLASSICAL ACTION FOR THE CHAIN $S = \int L(\dot{\phi}_n, \phi_n)$ LEADS TO

$$\frac{d}{dt}(\partial_{\dot{\phi}_n} L) - \partial_{\phi_n} L = 0$$

WITH $\partial_{\dot{\phi}_n} L = m\dot{\phi}_n$ AND $\partial_{\phi_n} L = -k(\phi_n - \phi_{n+1}) + - k(\phi_n - \phi_{n-1})$ WE OBTAIN THE DISCRETE CLASSICAL EQ. OF MOTION WE HAVE ALREDY SEEN

$$m\ddot{\phi}_n = -k(\phi_n - \phi_{n+1}) - k(\phi_n - \phi_{n-1})$$ FOR EACH n. THESE EQUATIONS DESCRIBE THE NORMAL VIBRATION MODES OF THE SYSTEM. SETTING $\phi_n(t) = \phi_n e^{-i\Omega t}$ THE CORRESPONDING

ALGEBRICAL EQ FOR EACH n IS

$$\left(-m\Omega^2+2k\right)\phi_n - k\left(\phi_{n+1}+\phi_{n-1}\right)=0$$

THIS EQS HAVE WAVE-LIKE SOLUTIONS (NORMAL MODES) OF THE FORM $\phi_n=\frac{1}{\sqrt{N}}e^{iKna}$

• OBSERVATION. HERE k IS THE SPRING CONSTANT, K IS THE WAVE NUMBER ($K=|\bar{K}|$ WHERE $\bar{K}$ IS THE WAVEVECTOR $\Rightarrow K=2\pi/a$) AND a IS THE LATTICE PARAMETER.

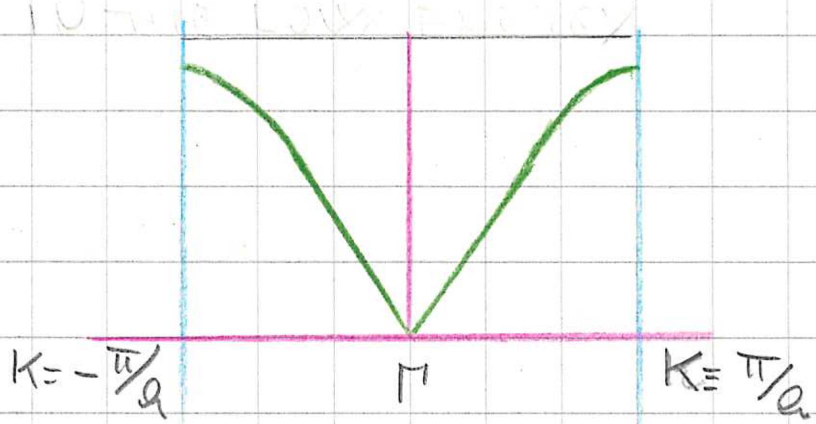
WITH THE PERIODIC BOUNDARY CONDITIONS $\phi_{n+N}=\phi_n$ WE HAVE $e^{iKNa}=1=e^{i(2\pi m)}$

$(m=0,1,2,\dots)$ $\Rightarrow$ $K=\frac{2\pi m}{Na}$ TAKES N DISCRETE VALUES. $\Rightarrow$ HENCE BY SUBSTITUTING INTO THE MOTION EQ WE OBTAIN

$$\left(-m\Omega^2+2k\right)=2k\cos(Ka) \Rightarrow$$

$$\Omega=\Omega_K=\sqrt{\frac{2k}{m}(1-\cos Ka)}=2\sqrt{\frac{k}{m}}\left|\sin\left(\frac{Ka}{2}\right)\right|$$

WHICH IS THE DISPERSION RELATION WE HAVE ALREADY SEEN FOR THE ACOUSTIC PHONONS.



FOR $K \to 0$ (LOW ENERGY RANGE)

$$\Omega_K \simeq V|K|$$

WHERE $V = a\sqrt{\frac{k}{m}}$ DENOTES THE SOUND VELOCITY OF THE COLLECTIVE WAVE-LIKE EXCITATION OF THE HARMONIC CHAIN.

IN THE CONTINUUM LIMIT (THE MASSES ARE NOT DISCRETE BUT A CONTINUUM MASS DISTRIBUTION) WE CAN DEFINE A MASS DENSITY $\rho = m/a$ (MASS PER UNIT LENGTH) AND $k_s = k/a$ SO THAT THE LAGRANGIAN IS

$$\mathcal{L}(\dot\phi, \phi) = \frac{\rho}{2}\dot\phi^2 - \frac{k_s a^2}{2}(\partial_x \phi)^2$$

LAGRANGIAN IN THE CONTINUUM LIMIT)

- OBSERVATION BY TURNING TO A CONTINUUM LIMIT WE HAVE SUCCEEDED IN ABANDONING THE N-POINT PARTICLE DESCRIPTION IN FAVOR OF ONE INVOLVING A SET OF CONTINUOS DEGREE OF FREEDOM, $\phi(x)$ KNOWN AS CLASSICAL FIELD.

WE CAN NOW USE THE CONVENTIONAL "CANONICAL QUANTIZATION PROCEDURE" THAT RECALLING THAT FOR A POINT PARTICLE MECHANICS WAS 1- DEFINITION OF THE CANONICAL MOMENTUM $p = \partial_{\dot x} \mathcal{L}(\dot x, x)$

(2) CONSTRUCT THE HAMILTONIAN

$$\mathcal{H}(x,p) = p\dot{x} - \mathcal{L}(\dot{x},x)$$

(3) PROMOTE THE CONJUGATE COORDINATES x, p TO OPERATORS WITH CANONICAL COMMUTATION RELATIONS

$$[\hat{p},\hat{x}] = -i\hbar$$

CANONICAL QUANTIZATION PROCEDURE FOR CONTINUUM THEORY FOLLOWS THE SAME PATH

(1) DEFINE THE CANONICAL MOMENTUM

$$\pi = \partial_{\dot{\phi}}\mathcal{L}(\dot{\phi},\phi) = \rho\dot{\phi}$$

(2) CONSTRUCT THE HAMILTONIAN

$$\hat{H}(\phi,\pi) \equiv \int dx\, \mathcal{H}(\phi,\pi)$$

WHERE THE HAMILTONIAN DENSITY

$$\mathcal{H}(\phi,\pi) = \pi\dot{\phi} - \mathcal{L}(\dot{\phi},\phi) = \frac{1}{2\rho}\pi^2 + \frac{k_s a^2}{2}(\partial_x\phi)^2$$

(3) PROMOTE FIELD $\phi(x)$ AND $\pi(x)$ TO OPERATORS WITH CANONICAL COMMUTATION RELATIONS

$$[\hat{\pi}(x),\hat{\phi}(x')] = -i\hbar\,\delta(x-x')$$

{LENGTH OF THE STRING

$$\Rightarrow \hat{H} = \int_0^L dx\left[\frac{1}{2\rho}\hat{\pi}^2 + \frac{k_s a^2}{2}(\partial_x\hat{\phi})^2\right]$$

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WHICH IN THE FOURIER REPRESENTATION

$$\hat{\phi}(x) = \frac{1}{L^{1/2}}\sum_k' e^{ikx}\hat{\phi}_k$$

(WE HAVE OMITTED HERE THE CALCULUS)

GIVES
$$\hat{H} = \sum_k{}' \left[\frac{1}{2\rho} \hat{\Pi}_k \hat{\Pi}_{-k} + \frac{1}{2} \rho \Omega_k^2 \hat{\phi}_k \hat{\phi}_{-k} \right]$$

THIS $\hat{H}$ DESCRIBES SET OF QUANTUM HARMONIC OSCILLATOR.

INSPIRED BY LADDER OPERATOR FORMALISM WE CAN DEFINE THE FOLLOWING OPERATORS

$$\hat{a}_k \equiv \sqrt{\frac{m\Omega_k}{2\hbar}} \left(\hat{\phi}_k + \frac{i}{m\Omega_k} \hat{\Pi}_{-k} \right)$$

$$\hat{a}^+_{k'} \equiv \sqrt{\frac{m\Omega_k}{2\hbar}} \left(\hat{\phi}_{-k} - \frac{i}{m\Omega_k} \hat{\Pi}_k \right)$$

THESE LEDDER OPERATORS OBEY THE COMMUTATION RELATION

$$\left[\hat{a}_k, \hat{a}^+_{k'}\right] = \delta_{kk'}, \quad \left[\hat{a}_k, \hat{a}_{k'}\right] = \left[\hat{a}^+_k, \hat{a}^+_{k'}\right] = 0$$

AND THE HAMILTONIAN ASSUMES THE DIAGONAL FORM
$$\hat{H} = \sum_k{}' \hbar\Omega_k \left(\hat{a}^+_k \hat{a}_k + \frac{1}{2} \right)$$

- OBSERVATION LOW ENERGY EXCITATION OF DISCRETE ATOMIC CHAIN BEHAVE AS DISCRETE PARTICLES (EVEN IF THEY DESCRIBE THE COLLECTIVE MOTION OF AN INFINITE NUMBER OF "FUNDAMENTAL DEGREES OF FREEDOM)

DESCRIBING OSCILLATOR WAVE-LIKE MODES,

- THESE PARTICLE LIKE EXCITATIONS, KNOWN AS PHONONS ARE CHARACTERIZED BY A WAVEVECTOR $\bar{K}$ AND HAVE A LINEAR DISPERSION $\Omega_K = v|\bar{K}|$.