TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

SFB 1143

Solid State Theory (SS2020)

Lecture 2: Lattice dynamics

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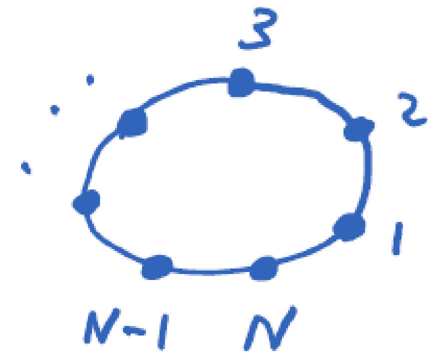
§ 1.1 Classical monoatomic chain

- Last lecture: Classical theory of a monoatomic chain

$$H = \sum_{i=1}^{N} \frac{1}{2} M \dot{u}_i^2 + V(\{u_i\})$$

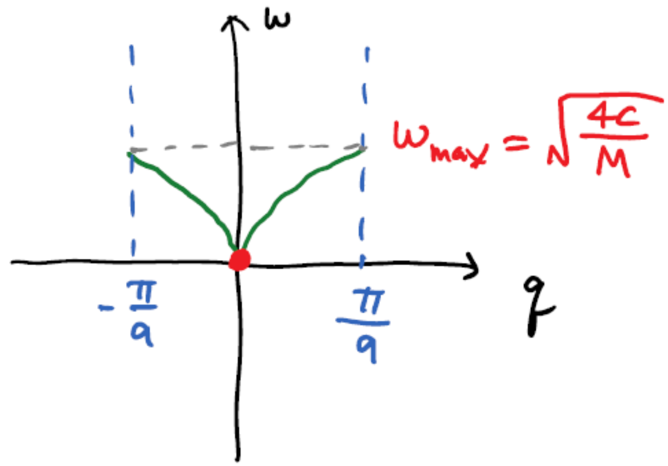
$$\frac{1}{2}\sum_{i,j=1}^{N} D_{ij} u_i u_j + \cdots$$



Running wave solution:

$$u_j(t) = A\, e^{i(qja - \omega t)}$$

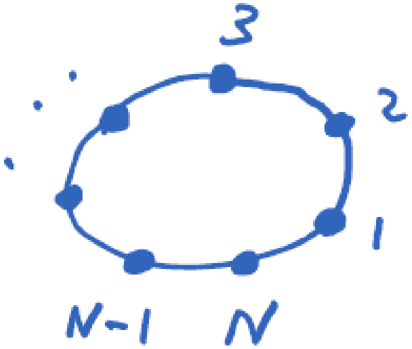
$$\omega(q) = \sqrt{\frac{4C}{M}}\left|\sin\frac{qa}{2}\right|$$



§ 1.2 Quantum monoatomic chain

- Today: Quantum theory of a monoatomic chain

$$H = \sum_{j=1}^{N} \frac{P_j^2}{2M} + \frac{1}{2} c \sum_{j=1}^{N} (u_{j+1} - u_j)^2$$



Commutation relations:

$$\begin{cases} [u_j, u_\ell] = [P_j, P_\ell] = 0 \\ [u_j, P_\ell] = i\hbar \delta_{j\ell} \end{cases}$$

Coupled harmonic oscillators!

§ 1.2 Quantum monoatomic chain

- General strategy: decouple the oscillators via canonical transformations

$$P = \begin{pmatrix} P_1 \\ P_2 \\ \vdots \\ P_N \end{pmatrix} \qquad u = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{pmatrix}$$

$$H = \sum_{j=1}^{N} \frac{P_j^2}{2M} + \frac{1}{2} C \sum_{j,l=1}^{N} u_j D_{jl} u_l$$

$$= \frac{1}{2M} P^T P + \frac{1}{2} C\, u^T D u$$

Diagonalize D :

real, symmetric matrix

$$O^T D O = \Lambda = \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_N \end{pmatrix}$$

orthogonal matrix $O^T O = O O^T = 1_{N \times N}$

§ 1.2 Quantum monoatomic chain

- General strategy: decouple the oscillators via canonical transformations

$$P = \begin{pmatrix} P_1 \\ P_2 \\ \vdots \\ P_N \end{pmatrix} \qquad u = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{pmatrix}$$

$$H = \frac{1}{2M} P^T O^T \underbrace{O P}_{\equiv P'} + \frac{1}{2} C\, u^T O^T \Lambda \underbrace{O u}_{\equiv u'}$$

$$= \frac{1}{2M} P'^T P' + \frac{1}{2} C\, u'^T \Lambda u'$$

$$= \sum_{q=1}^{N} \left(\frac{1}{2M} P_q'^2 + \frac{1}{2} C \lambda_q u_q'^2 \right)$$

$[u_p', P_q'] = i\hbar\delta_{pq}$ $\quad [u_p', u_q'] = [P_p', P_q'] = 0$ Decoupled harmonic oscillators!

§ 1.2 Quantum monoatomic chain

- Proof of the canonical commutation relation:

$$\begin{cases} u'_p = \sum_{j=1}^{N} O_{pj} u_j \\ p'_q = \sum_{j=1}^{N} O_{qj} p_j \end{cases} \Rightarrow$$

$$\begin{aligned}
[u'_p, p'_q] &= \sum_{j,l=1}^{N} O_{pj} O_{ql} \underbrace{[u_j, p_l]}_{= i\hbar \delta_{jl}} \\
&= i\hbar \sum_{j=1}^{N} O_{pj} \underbrace{O_{qj}}_{= O^T_{jq}} \\
&= i\hbar (\underbrace{O O^T}_{= I_{N\times N}})_{pq} \\
&= i\hbar \delta_{pq}
\end{aligned}$$

§ 1.2 Quantum monoatomic chain

- Proof of the canonical commutation relation:

$$\begin{cases} u'_p = \sum_{j=1}^{N} O_{pj} u_j \\ P'_q = \sum_{j=1}^{N} O_{qj} P_j \end{cases} \Rightarrow$$

$$\begin{aligned}
[u'_p, P'_q] &= \sum_{j,\ell=1}^{N} O_{pj} O_{q\ell} \underbrace{[u_j, P_\ell]}_{= i\hbar \delta_{j\ell}} \\
&= i\hbar \sum_{j=1}^{N} O_{pj} \underbrace{O_{qj}}_{= O^T_{jq}} \\
&= i\hbar \, (\underbrace{O O^T}_{= I_{N\times N}})_{pq} \\
&= i\hbar \, \delta_{pq}
\end{aligned}$$

$$[u'_p, u'_q] = [P'_p, P'_q] = 0$$

N decoupled harmonic oscillators !

§ 1.2 Quantum monoatomic chain

- Review: single quantum harmonic oscillator:

$$H = \frac{1}{2M}P^2 + \frac{1}{2}M\omega^2 x^2$$

$$= \frac{1}{2}\hbar\omega\left(\frac{1}{M\omega\hbar}P^2 + \frac{M\omega}{\hbar}x^2\right)$$

$$= \frac{1}{2}\hbar\omega\left(\frac{\ell_0^2}{\hbar^2}P^2 + \frac{1}{\ell_0^2}x^2\right)$$

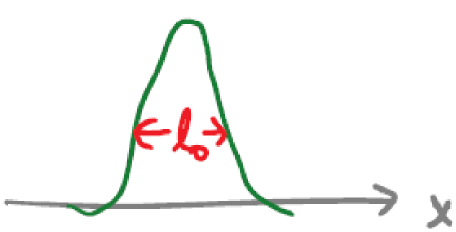
Length unit:

$$\ell_0 = \sqrt{\frac{\hbar}{M\omega}}$$

- Ground state in real space: Gaussian wave packet

⇨ Atoms vibrate even at zero temperature.

(zero-point motion due to Heisenberg's uncertainty principle)



§ 1.2 Quantum monoatomic chain

- Bosonic operators:

$$a^+ , \ a \qquad [a, a^+] = 1$$

Hilbert space: $|0\rangle$ ("vacuum", $a|0\rangle = 0$)

$$|n\rangle = \frac{1}{n!}(a^+)^n|0\rangle , \quad n = 0, 1, 2, \cdots$$

$$\langle n|n'\rangle = \delta_{nn'}$$

$$a^\dagger a|n\rangle = n|n\rangle$$

Boson particle number

§ 1.2 Quantum monoatomic chain

- Solving the quantum harmonic oscillator via boson mapping:

$$\boxed{\begin{aligned} x &= \frac{1}{\sqrt{2}} l_0 (a + a^\dagger) \\ p &= \frac{-i}{\sqrt{2}} \frac{\hbar}{l_0} (a - a^\dagger) \end{aligned}}$$

$$\begin{aligned} [x, p] &= \frac{-i}{2}\hbar \, [a + a^\dagger, a - a^\dagger] \\ &= \frac{-i}{2}\hbar \, (-1 - 1) \\ &= i\hbar \quad \checkmark \end{aligned}$$

$$\begin{aligned} \Rightarrow \quad H &= \frac{1}{2}\hbar\omega \left(\frac{l_0^2}{\hbar^2} p^2 + \frac{1}{l_0^2} x^2 \right) \\ &= \frac{1}{2}\hbar\omega \left[-\frac{1}{2} (a - a^\dagger)^2 + \frac{1}{2} (a + a^\dagger)^2 \right] \end{aligned}$$

$$(a - a^\dagger)^2 = (a - a^\dagger)(a - a^\dagger) = a^2 + (a^\dagger)^2 - a a^\dagger - a^\dagger a$$

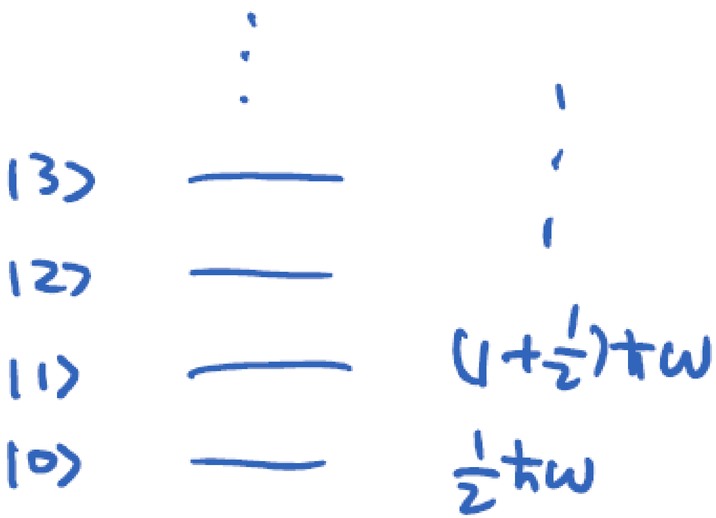
$$(a + a^\dagger)^2 = (a + a^\dagger)(a + a^\dagger) = a^2 + (a^\dagger)^2 + a a^\dagger + a^\dagger a$$

$$\begin{aligned} &= \frac{1}{2}\hbar\omega \, (a a^\dagger + a^\dagger a) \\ &= \hbar\omega \, \left(a^\dagger a + \frac{1}{2}\right) \end{aligned}$$

§ 1.2 Quantum monoatomic chain

- Solving the quantum harmonic oscillator via boson mapping:

$$H|n\rangle = \hbar\omega\left(a^{\dagger}a+\tfrac{1}{2}\right)|n\rangle$$
$$= \hbar\omega\left(n+\tfrac{1}{2}\right)|n\rangle$$



Create excitations by adding bosons

§ 1.2 Quantum monoatomic chain

- Now we go back to the quantum monoatomic chain:

$$H = \sum_{j=1}^{N} \frac{P_j^2}{2M} + \frac{1}{2} c \sum_{j=1}^{N} (u_{j+1} - u_j)^2$$

- The Fourier transform and its inverse are canonical transformations:

$$\begin{cases} u_j = \frac{1}{\sqrt{N}} \sum_q e^{iqja} u_q \\ u_q = \frac{1}{\sqrt{N}} \sum_j e^{-iqja} u_j \end{cases}$$

$q \in FBZ$

$q = 0, \pm \frac{2\pi}{Na}, \ldots$

$$\begin{cases} P_j = \frac{1}{\sqrt{N}} \sum_q e^{-iqja} P_q \\ P_q = \frac{1}{\sqrt{N}} \sum_j e^{iqja} P_j \end{cases}$$

Note that $u_{-q} = u_q^\dagger$

$P_{-q} = P_q^\dagger$

§ 1.2 Quantum monoatomic chain

Proof:

$$[u_q, P_{q'}] = \frac{1}{N}\sum_{j,l} e^{-iqja+iq'la}\underbrace{[u_j, P_l]}_{=i\hbar\delta_{jl}}$$

$$= i\hbar\frac{1}{N}\sum_{j} e^{i(q'-q)ja}$$

$$= i\hbar\,\delta_{q',q}$$

Useful identities:

$$\frac{1}{N}\sum_{j=1}^{N} e^{i(q'-q)ja} = \delta_{q'q} \qquad \frac{1}{N}\sum_{q\in\mathrm{FBZ}} e^{iq(j-j')a} = \delta_{jj'}$$

§ 1.2 Quantum monoatomic chain

- Solving the quantum monoatomic chain via boson mapping:

$$H = \sum_j \frac{P_j^2}{2M} + \frac{1}{2} c \sum_j (u_{j+1} - u_j)^2$$

$$= \sum_j \frac{P_j^2}{2M} + \frac{1}{2} c \sum_j (2u_j^2 - u_{j+1}u_j - u_{j-1}u_j)$$

$$= \frac{1}{N} \sum_j \sum_{q,q'} \frac{1}{2M} P_q P_{q'} e^{-i(q+q')ja} \Leftarrow \frac{1}{N}\sum_j e^{i(q+q')ja} = \delta_{q',-q}$$

$$+ \frac{1}{2} c \frac{1}{N} \sum_j \sum_{q,q'} u_q u_{q'} \Big[2e^{i(q+q')ja} - e^{iq(j+1)a + iq'ja} - e^{iq(j-1)a + iq'ja} \Big]$$

$$= \sum_q \frac{1}{2M} P_q P_{-q} + \frac{1}{2} \sum_q u_q u_{-q} (2 - e^{iqa} - e^{-iqa})$$

$$= \sum_q \left(\frac{1}{2M} P_q P_{-q} + 2c \sin^2\frac{qa}{2}\, u_q u_{-q} \right)$$

§ 1.2 Quantum monoatomic chain

- Solving the quantum monoatomic chain via boson mapping:

$$H = \sum_q \left(\frac{1}{2M} P_q P_{-q} + \frac{1}{2} M \omega_q^2 u_q u_{-q} \right)$$

$$\omega_q = \sqrt{\frac{4C}{M}} \left| \sin \frac{qa}{2} \right| \Leftarrow$$ frequency from classical E.O.M !

$$H = \sum_q H(q), \quad \text{where} \quad [H(q), H(q')] = 0$$

Each $H(q)$ describes a harmonic oscillator.

$q \in FBZ \longrightarrow N$ independent harmonic oscillators

§ 1.2 Quantum monoatomic chain

- Solving the quantum monoatomic chain via boson mapping:

$$H = \sum_q \left(\frac{1}{2M} P_q P_{-q} + \frac{1}{2} M \omega_q^2 u_q u_{-q} \right)$$

Last canonical transformation to diagonalize the Hamiltonian:

$$a_q = \sqrt{\frac{m\omega_q}{2\hbar}}\, u_q + i\sqrt{\frac{1}{2M\hbar\omega_q}}\, P_{-q}$$

$$a_q^+ = \sqrt{\frac{m\omega_q}{2\hbar}}\, u_{-q} - i\sqrt{\frac{1}{2M\hbar\omega_q}}\, P_q$$

Check: $[a_q, a_{q'}] = [a_q^+, a_{q'}^+] = 0$

$[a_q, a_{q'}^+] = \delta_{qq'}$

§ 1.2 Quantum monoatomic chain

- Solving the quantum monoatomic chain via boson mapping:

$$H = \sum_q \left(\frac{1}{2M} P_q P_{-q} + \frac{1}{2} M \omega_q^2 u_q u_{-q} \right)$$

Last canonical transformation to diagonalize the Hamiltonian:

$$a_q = \sqrt{\frac{m\omega_q}{2\hbar}}\, u_q + i \sqrt{\frac{1}{2M\hbar\omega_q}}\, P_{-q}$$

$$a_q^{+} = \sqrt{\frac{m\omega_q}{2\hbar}}\, u_{-q} - i \sqrt{\frac{1}{2M\hbar\omega_q}}\, P_q$$

One minor subtlety: $q = 0$ has to be treated with care ($a_{q=0}$ and $a_{q=0}^{\dagger}$ not well defined in the above form due to $\omega_{q=0} = 0$). Note that $H(q = 0) = \frac{P_{q=0}^2}{2M}$, which is the kinetic energy corresponding to the "center-of-mass".

§ 1.2 Quantum monoatomic chain

- Solving the quantum monoatomic chain via boson mapping:

$$H = \sum_q \left(\frac{1}{2M} P_q P_{-q} + \frac{1}{2} M \omega_q^2 u_q u_{-q} \right)$$

Last canonical transformation to diagonalize the Hamiltonian:

$$a_q = \sqrt{\frac{m\omega_q}{2\hbar}}\, u_q + i\sqrt{\frac{1}{2M\hbar\omega_q}}\, P_{-q}$$

$$a_q^+ = \sqrt{\frac{m\omega_q}{2\hbar}}\, u_{-q} - i\sqrt{\frac{1}{2M\hbar\omega_q}}\, P_q$$

Inverse transformation:

$$\begin{cases} u_q = \sqrt{\frac{\hbar}{2M\omega_q}}\,(a_q + a_{-q}^+) \\ P_q = (-i)\sqrt{\frac{M\hbar\omega_q}{2}}\,(a_{-q} - a_q^+) \end{cases}$$

§ 1.2 Quantum monoatomic chain

- Solving the quantum monoatomic chain via boson mapping:

$$H = \sum_q \left(\frac{1}{2M} P_q P_{-q} + \frac{1}{2} M \omega_q^2 u_q u_{-q} \right)$$

The point of designing the canonical transformation is to eliminate the "off-diagonal" terms in H:

$$\frac{1}{2M} P_q P_{-q} = \frac{1}{2M} (-1) \frac{M\hbar\omega_q}{2} (a_{-q} - a_q^{\dagger})(a_q - a_{-q}^{\dagger})$$

$$= -\frac{1}{4}\hbar\omega_q \left(a_{-q} a_q + a_q^{\dagger} a_{-q}^{\dagger} - a_q^{\dagger} a_q - a_{-q} a_{-q}^{\dagger} \right)$$

$$\frac{1}{2} M \omega_q^2 u_q u_{-q} = \frac{1}{2} M \omega_q^2 \frac{\hbar}{2M\omega_q} (a_q + a_{-q}^{\dagger})(a_{-q} + a_q^{\dagger})$$

$$= \frac{1}{4}\hbar\omega_q \left(a_q a_{-q} + a_{-q}^{\dagger} a_q^{\dagger} + a_{-q}^{\dagger} a_{-q} + a_q a_q^{\dagger} \right)$$

§ 1.2 Quantum monoatomic chain

- Solving the quantum monoatomic chain via boson mapping:

$$H = \sum_q \left(\frac{1}{2M} P_q P_{-q} + \frac{1}{2} M \omega_q^2 u_q u_{-q} \right)$$

The point of designing the canonical transformation is to eliminate the "off-diagonal" terms in H:

$$aa^\dagger = [a, a^\dagger] + a^\dagger a = a^\dagger a + 1$$

$$\frac{1}{2M} P_q P_{-q} = \frac{1}{2M}(-1)\frac{M\hbar\omega_q}{2}\left(a_{-q} - a_q^\dagger\right)\left(a_q - a_{-q}^\dagger\right)$$

$$= -\frac{1}{4}\hbar\omega_q \left(\cancel{a_{-q} a_q + a_q^\dagger a_{-q}^\dagger} - a_q^\dagger a_q - a_{-q} a_{-q}^\dagger \right)$$

$$\frac{1}{2} M \omega_q^2 u_q u_{-q} = \frac{1}{2} M \omega_q^2 \frac{\hbar}{2M\omega_q}\left(a_q + a_{-q}^\dagger\right)\left(a_{-q} + a_q^\dagger\right)$$

$$= \frac{1}{4}\hbar\omega_q \left(\cancel{a_q a_{-q} + a_{-q}^\dagger a_q^\dagger} + a_{-q}^\dagger a_{-q} + a_q a_q^\dagger \right)$$

§ 1.2 Quantum monoatomic chain

- Solving the quantum monoatomic chain via boson mapping:

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

$$H \left| n_{q=0}, \cdots, n_{q=\frac{\pi}{a}} \right\rangle = \underbrace{\sum_q \hbar\omega_q \left(n_q + \frac{1}{2} \right)}_{E = \sum_q \hbar\omega_q \left(n_q + \frac{1}{2} \right)} \left| n_{q=0}, \cdots, n_{q=\frac{\pi}{a}} \right\rangle$$

$$\left| n_{q=0}, n_{q=\frac{2\pi}{Na}}, n_{q=-\frac{2\pi}{Na}}, \cdots, n_{q=\frac{\pi}{a}} \right\rangle$$

$$= \frac{1}{\sqrt{n_{q=0}! \cdots n_{q=\frac{\pi}{a}}!}} \left(a_{q=0}^{+} \right)^{n_{q=0}} \left(a_{q=\frac{2\pi}{Na}}^{+} \right)^{n_{q=\frac{2\pi}{Na}}} \cdots \left(a_{q=\frac{\pi}{a}}^{+} \right)^{n_{q=\frac{\pi}{a}}} |0\rangle$$

§ 1.2 Quantum monoatomic chain

- Solving the quantum monoatomic chain via boson mapping:

$$\boxed{H = \sum_q \hbar\omega_q \left(a_q^\dagger a_q + \frac{1}{2} \right)}$$

$$H \,|\, n_{q=0}, \cdots, n_{q=\frac{\pi}{a}} \rangle = \underbrace{\sum_q \hbar\omega_q \left(n_q + \frac{1}{2} \right)}_{E = \sum_q \hbar\omega_q \left(n_q + \frac{1}{2} \right)} \,|\, n_{q=0}, \cdots, n_{q=\frac{\pi}{a}} \rangle$$

- Excitations correspond to the creation of bosonic modes $a_q^\dagger$.
  These are quantized collective excitations, called "phonons".

§ 1.2 Quantum monoatomic chain

- Solving the quantum monoatomic chain via boson mapping:

$$\boxed{H = \sum_q \hbar\omega_q \left(a_q^\dagger a_q + \frac{1}{2} \right)}$$

$$H \left| n_{q=0}, \cdots, n_{q=\frac{\pi}{a}} \right\rangle = \underbrace{\sum_q \hbar\omega_q \left(n_q + \frac{1}{2} \right)}_{E = \sum_q \hbar\omega_q \left(n_q + \frac{1}{2} \right)} \left| n_{q=0}, \cdots, n_{q=\frac{\pi}{a}} \right\rangle$$

Here we abused the notation a bit to include $q = 0$, because it can be viewed as an artifact of PBC ("center-of-mass" momentum is conserved). Note that the boundary condition shouldn't affect the "bulk" physics if the number of atoms is large (thermodynamic limit $N \to \infty$).

§ 1.2 Quantum monoatomic chain

- Summary:

  - We have quantized the monoatomic chain. Apparently, the system becomes decoupled harmonic oscillators after successive canonical transformations.

    Useful technique for other “quadratic” Hamiltonians

  - The dispersion relation is the same as the classical one.

    Generally true for other lattice vibration problems under the harmonic approximation (dispersion comes from the eigenvalues of the dynamical matrix)

  - The elastic waves in the classical case become collective excitations (“phonon”) in the quantum case.