TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

SFB 1143

Solid State Theory (SS2020)

Lecture 1: General introduction + Lattice dynamics

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April 8th, 2020

Time and format

- Lecture/tutorial: Wednesday 14:50 – 16:20
  Thursday 13:00 – 14:30
- Office hours: Friday 13:00 – 14:00
  + appointment

Likely shorter with Zoom (< 60 mins)

- If the network bandwidth is not enough for live mode, we distribute the lecture notes in advance and discuss in 2 – 3 smaller groups.
- After fixing the format, a schedule with course outline will be uploaded in the course webpage.

Course webpage: https://tu-dresden.de/mn/physik/itp/ket/studium/lehre/sst_ss20

Exercise and oral exam

Exercise:

- There will be five exercises. We will discuss them during the tutorials.
- There is no written exam. For Bachelor and Master students who need a grade, it's required to correctly finish at least 60% of the exercises. Send your solutions to me by email.

Oral exam:

- For Master students, this course can be chosen as one of the two oral exam subjects for "Vertiefung: Theoretische Physik".
- Doctoral candidates may take the oral exam in replacement for the Rigorosum or choose this course to be examined in the Rigorosum.

Reference

- U. Rössler, Solid State Theory, Springer (2009).
- G. Grosso & G. P. Parravicini, Solid State Physics, Academic Press (2000).
- N. W. Ashcroft & N. D. Mermin, Solid State Physics, Holt, Rinehart and Winston (1976).
- G. Czycholl, Theoretische Festkörperphysik, Springer (2004).
- O. Madelung, Introduction to Solid-State Theory, Springer (1981).

There are many good books, but you are encourage to use the ones with second quantization formulations…

Notes from SS2019: https://tu-dresden.de/mn/physik/itp/ket/studium/lehre/sst_ss19

Covered topics

- Lattice vibrations and phonons
- Free and interacting electron gases
- Energy band theory
- Transport theory
- Electrons in a magnetic field and quantum Hall physics
- Quantum magnetism (or superconductivity, topological insulators)
- …

Concepts + models + techniques

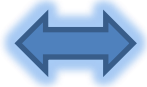
§ 0. General Introduction

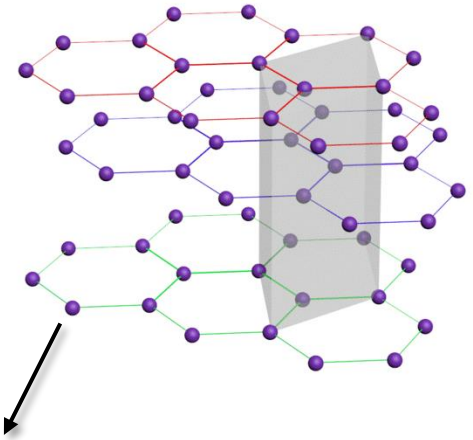
Target: solids formed by large number of atoms

$\sim 10^{23}$

- Due to inter-atomic interactions (chemical bonds), solids often show periodic structures.

Graphite:





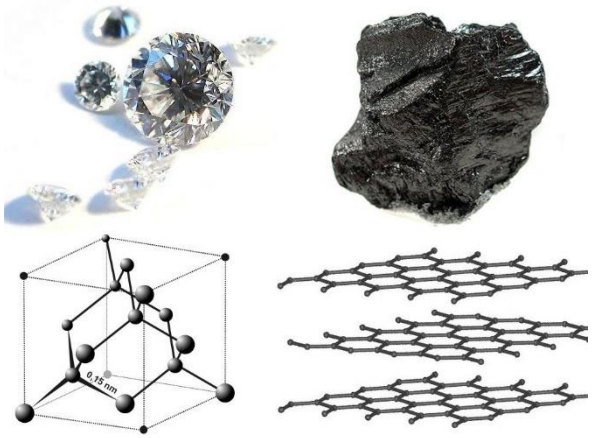
Carbon ($1s^2 2s^2 2p^2$)

Figures from Wikipedia and Wikimedia

§ 0. General Introduction

- Properties of the solids depend on
  - ➢ type of atoms
  - ➢ how atoms form periodic structure
- Due to inter-atomic interactions, it is a many-body problem.
- As a consequence, solids exhibit many properties which are not enjoyed by single (or few) atoms.

"More is different!" – Philip W. Anderson



diamond graphite

Figure from Wikimedia

§ 0. General Introduction

- We are interested in understanding the physical properties of solids, such as electronic, magnetic, optical properties.
- The theoretical understanding is ideally established from first principles, i.e. quantum and statistical mechanics:

(Almost) zero temperature: $H|\psi\rangle = E|\psi\rangle$ → ground state

Finite temperature: $Z = \mathrm{Tr}(e^{-\beta H})$ → partition function; $\beta = \frac{1}{k_B T}$

§ 0. General Introduction

- Solid = ions + electrons
- Hamiltonian = kinetic energy terms + interaction terms

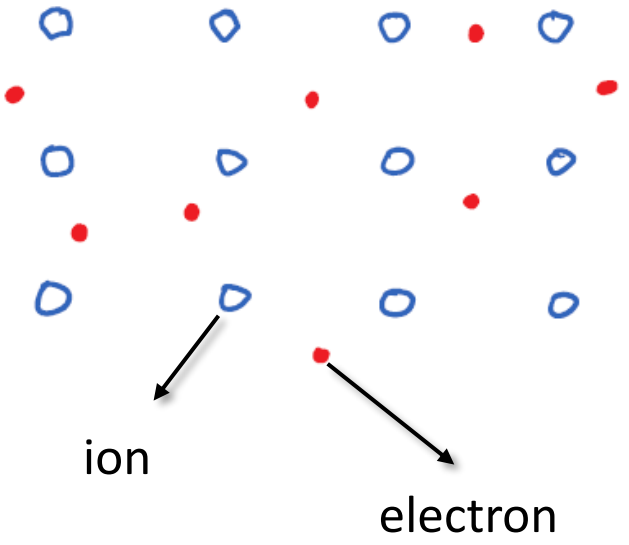
$$H = H_{ion} + H_{el} + H_{el\text{-}ion}$$

$$H_{ion} = \sum_{i=1}^{N_I} \frac{\vec{P}_i^{\,2}}{2M_i} + \frac{1}{2} \sum_{i \neq i'}^{N_I} V(\vec{R}_i - \vec{R}_{i'})$$

$$V(\vec{R}_i - \vec{R}_{i'}) = \frac{Z_i Z_i e^2}{4\pi\varepsilon_0 |\vec{R}_i - \vec{R}_{i'}|}$$

$$H_{el} = \sum_{j=1}^{N_e} \frac{\vec{P}_j^{\,2}}{2m} + \frac{1}{2} \sum_{j \neq j'}^{N_e} \frac{e^2}{4\pi\varepsilon_0 |\vec{r}_j - \vec{r}_{j'}|}$$

$$H_{el\text{-}ion} = -\sum_{i=1}^{N_I} \sum_{j=1}^{N_e} \frac{Z_i e^2}{4\pi\varepsilon_0 |\vec{R}_i - \vec{r}_j|}$$



§ 0. General Introduction

- Schrödinger's equation:

$$H\,\psi(\vec{r}_1,\dots,\vec{r}_{N_e};\vec{R}_1,\dots,\vec{R}_{N_I}) = E\,\psi(\vec{r}_1,\dots,\vec{r}_{N_e};\vec{R}_1,\dots,\vec{R}_{N_I})$$

No hope to solve it exactly!

$N_e,\ N_I \sim 10^{23}$

Quantum Mechanics of Many-Electron Systems.

By P. A. M. Dirac, St. John's College, Cambridge.

(Communicated by R. H. Fowler, F.R.S.—Received March 12, 1929.)

§ 1. *Introduction.*

The general theory of quantum mechanics is now almost complete, the imperfections that still remain being in connection with the exact fitting in of the theory with relativity ideas. These give rise to difficulties only when high-speed particles are involved, and are therefore of no importance in the consideration of atomic and molecular structure and ordinary chemical reactions, in which it is, indeed, usually sufficiently accurate if one neglects relativity variation of mass with velocity and assumes only Coulomb forces between the various electrons and atomic nuclei. The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.

§ 0. General Introduction

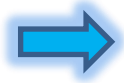
- Schrödinger's equation:

$$H\,\psi(\vec{r}_1,\dots,\vec{r}_{N_e};\vec{R}_1,\dots,\vec{R}_{N_I}) = E\,\psi(\vec{r}_1,\dots,\vec{r}_{N_e};\vec{R}_1,\dots,\vec{R}_{N_I})$$

No hope to solve it exactly!

$N_e,\ N_I \sim 10^{23}$

- What can we do?
  - Ignore (or average over) some terms in H
  - Treat some terms as perturbations
  - Use symmetry (translation, rotation, …)



Require physical considerations!

§ 1. Lattice dynamics

- We focus on ions first:

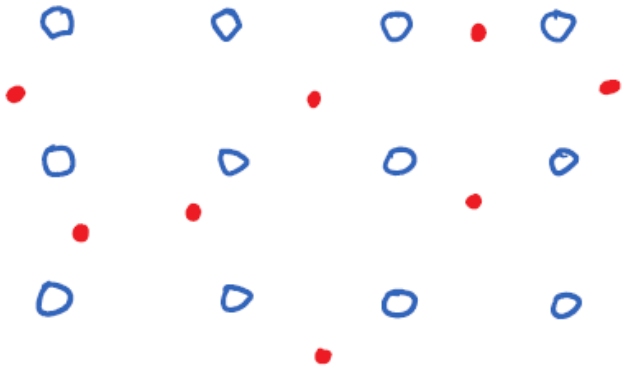
$$H = H_{ion} + H_{el} + H_{el\text{-}ion}$$

$$H_{ion} = \sum_{i=1}^{N_I} \frac{\vec{P}_i^{\,2}}{2M_i} + \frac{1}{2}\sum_{i\neq i'}^{N_I} V(\vec{R}_i - \vec{R}_{i'})$$

$$\| \quad \frac{Z_i Z_i e^2}{4\pi\varepsilon_0 |\vec{R}_i - \vec{R}_{i'}|}$$

$$H_{el} = \sum_{j=1}^{N_e} \frac{\vec{P}_j^{\,2}}{2m} + \frac{1}{2}\sum_{j\neq j'}^{N_e} \frac{e^2}{4\pi\varepsilon_0 |\vec{r}_j - \vec{r}_{j'}|}$$

$$H_{el\text{-}ion} = -\sum_{i=1}^{N_I}\sum_{j=1}^{N_e} \frac{Z_i e^2}{4\pi\varepsilon_0 |\vec{R}_i - \vec{r}_j|}$$



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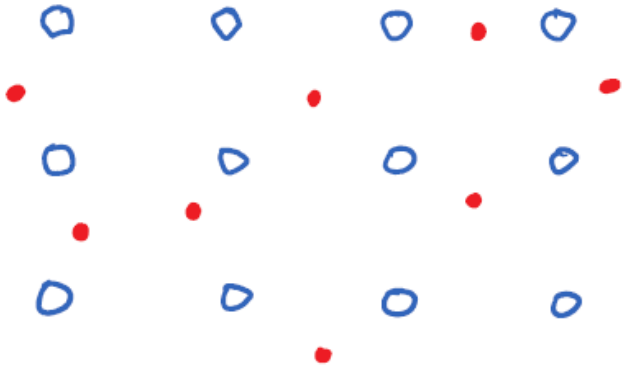

Let's assume that the electrons just provide a "background" for ion motions => average over electron coordinates

§ 1. Lattice dynamics

$$H_{ion} = \sum_{i=1}^{N_I} \frac{\vec{P}_i^{\,2}}{2M_i} + \frac{1}{2} \sum_{i \neq i'}^{N_I} V(\vec{R}_i - \vec{R}_{i'})$$

$$+ \varepsilon_{el\text{-}ion}(\{\vec{R}_i\})$$

$$\| $$

$$\langle H_{el\text{-}ion} \rangle_{el} = - \sum_{i=1}^{N_I} \sum_{j=1}^{N_e} \frac{z_i e^2}{4\pi\varepsilon_0} \left\langle \frac{1}{|\vec{R}_i - \vec{r}_j|} \right\rangle_{el}$$

$$\int d\vec{r}_1 \cdots d\vec{r}_{N_e}\, \rho_{el}(\vec{r}_1, \ldots, \vec{r}_{N_e}) \times \cdots$$

§ 1. Lattice dynamics

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$$\Rightarrow \quad \tilde{H}_{ion} = \sum_i \frac{\vec{p}_i^{\,2}}{2M_i} + \frac{1}{2} \sum_{i \neq j} \tilde{V}(\vec{R}_i - \vec{R}_j)$$

§ 1. Lattice dynamics

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"Dressed" potential

§ 1. Lattice dynamics

Effective problem for ions:

$$\frac{m_e}{M_i} \sim 10^{-3} \ll 1$$

$$\tilde{H}_{ion} = \sum_i \frac{\vec{p}_i^2}{2M_i} + \frac{1}{2}\sum_{i \neq j} \tilde{V}(\vec{R}_i - \vec{R}_j)$$

$$\tilde{H}_{ion}\psi_{ion}(\vec{R}_1, \dots, \vec{R}_{N_I}) = E_{ion}\psi_{ion}(\vec{R}_1, \dots, \vec{R}_{N_I})$$

More rigorous treatment: Born-Oppenheimer approximation

$$\psi(\vec{r}_1, \dots, \vec{r}_{N_e}; \vec{R}_1, \dots, \vec{R}_{N_I}) \approx \psi_{el}(\vec{r}_1, \dots, \vec{r}_{N_e})\psi_{ion}(\vec{R}_1, \dots, \vec{R}_{N_I})$$

$$H = H_{ion} + H_{el} + H_{ion-el}$$

§ 1. Lattice dynamics

Effective problem for ions:

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Still rather difficult to solve for general $\tilde{V}(\vec{R}_i - \vec{R}_j)$!

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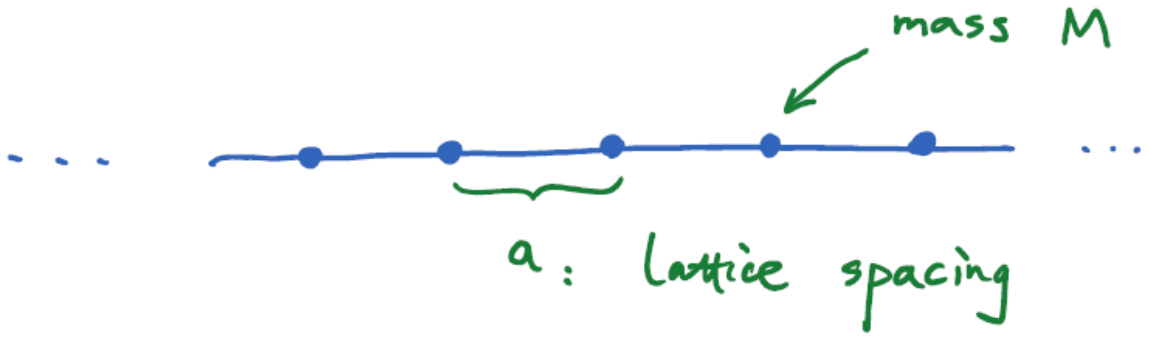
Still rather difficult to solve for general $\tilde{V}(\vec{R}_i - \vec{R}_j)$!

Physical consideration: ions vibrate near their equilibrium positions, so that $\tilde{V}(\vec{R}_i - \vec{R}_j)$ can be expanded around these equilibrium positions.

§ 1.1 Classical monoatomic chain

Let's gain some insights from the simplest case – monoatomic chain, and we start from the classical case first:

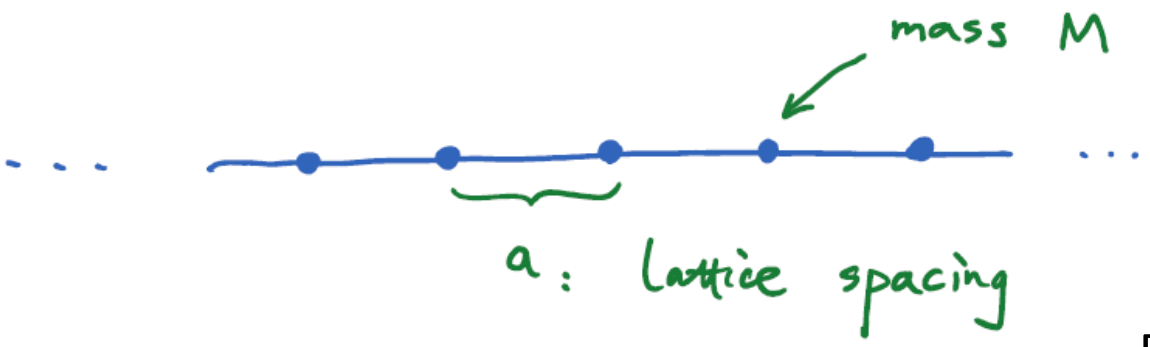


equilibrium position : ja $\quad j = 1, 2, \cdots, N$

displacement : u_j $\quad \Rightarrow R_j = ja + u_j$

physical requirement : $|u_j| \ll a$

§ 1.1 Classical monoatomic chain



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

Dynamical matrix:

$$D_{ij} = \frac{\partial^2 V}{\partial u_i \partial u_j}\Big|_0$$

$$V(\{u_i\}) \overset{|u_i| \ll a}{=} V_0 + \sum_{i=1}^{N} \left(\frac{\partial V}{\partial u_i}\right)\Big|_0 u_i + \frac{1}{2} \sum_{i,j=1}^{N} \left(\frac{\partial^2 V}{\partial u_i \partial u_j}\right)\Big|_0 u_i u_j$$

evaluated at $u_j = 0$

$= 0$ (equilibrium position minimizes V)

$+ O(u^3)$ dropped $\Rightarrow$ harmonic approximation

§ 1.1 Classical monoatomic chain

Force acting on the i-th ion:

$$F_i = -\frac{\partial V}{\partial u_i}$$

$$= -\frac{\partial}{\partial u_i}\left(V_0 + \frac{1}{2}\sum_{j,l=1}^{N} D_{jl}\, u_j u_l\right)$$

$$= -\sum_{j=1}^{N} D_{ij}\, u_j$$

Equation of motion (E.O.M.):

$$m\ddot{u}_i = -\sum_{j=1}^{N} D_{ij}\, u_j \qquad (i = 1, \ldots, N)$$

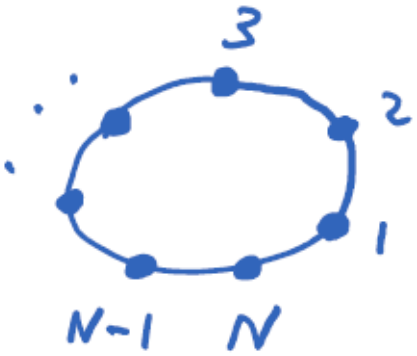
A set of N linearized differential equations, in principle the problem is solved

§ 1.1 Classical monoatomic chain

However, we haven't used the fact that all atoms should behave in the same way…

- Periodic boundary condition (PBC): $u_{N+j} = u_j$

  This imposes a translation symmetry!



$$D_{i+l,j+l} = D_{ij} \equiv D_{j-i}$$

$$\sum_{j=1}^{N} D_{ij} = 0$$

(global shift : $u_j = u \neq 0 \quad \forall j$)

no force: $0 = F_i = -u \sum_{j=1}^{N} D_{ij}$

§ 1.1 Classical monoatomic chain

Solving E.O.M. under PBC:

$$M\ddot{u}_i = F_i = -\sum_{j=1}^{N} D_{ij} u_j$$

Solution: $u_i = A_i e^{-i\omega t}$

→ time independent

$$\Rightarrow \quad -M\omega^2 A_i e^{-i\omega t} = -\sum_{j=1}^{N} D_{ij} A_j e^{-i\omega t}$$

(Linear equations determining A_j)

§ 1.1 Classical monoatomic chain

Ansatz: $A_j = A e^{iqja}$

$$\Rightarrow \quad M\omega^2 A e^{iqja} = \sum_{l=1}^{N} D_{jl} A e^{iqla}$$

Alternative way to find the above ansatz:

$$\sum_{j=1}^{N} D_{ij} A_j = M\omega^2 A_i$$

A_j and $M\omega^2$ are eigenvector and eigenvalue of the dynamical matrix D, respectively

$D_{ij} = D_{ji} = D_{j-i}$ => special case of the circulant matrix, whose eigenvectors take the above form (discrete Fourier transform)

§ 1.1 Classical monoatomic chain

Ansatz: $A_j = A\, e^{iqja}$

$$\Rightarrow \quad M\omega^2 A\, e^{iqja} = \sum_{l=1}^{N} D_{jl} A\, e^{iqla}$$

Dispersion relation:

$$\omega_q = \sqrt{\frac{1}{M}\sum_{l=1}^{N} D_{jl}\, e^{iq(l-j)a}} = \sqrt{\frac{D(q)}{M}}$$

$$D(q) \equiv \sum_{\delta} D_\delta\, e^{iq\delta}$$

translation symmetry

$$D_{jl} = D_{l-j} \equiv D_\delta$$

§ 1.1 Classical monoatomic chain

- Lattice vibration takes the form of a running wave!

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

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

- PBC only allows discrete wave vectors:

$$u_{j+N} = u_j \quad \Rightarrow \quad e^{iqNa} = 1$$

$$q = 0, \pm\frac{2\pi}{Na}, \pm\frac{4\pi}{Na}, \cdots, \pm\frac{(N-2)\pi}{Na}, \frac{\pi}{a} \quad (N \text{ even})$$

§ 1.1 Classical monoatomic chain

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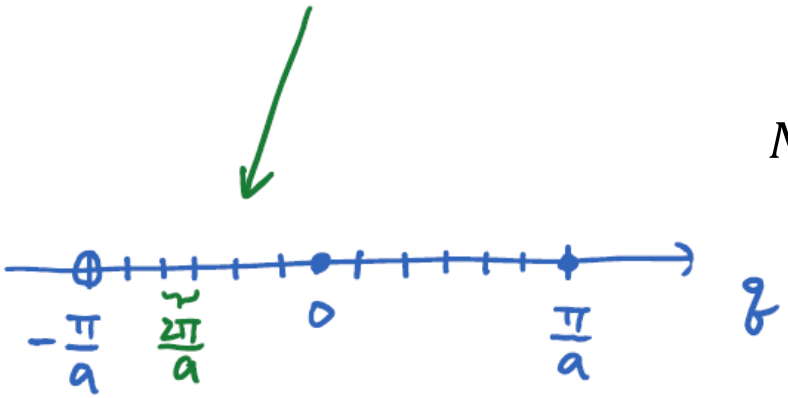
$$q = 0, \pm\frac{2\pi}{Na}, \pm\frac{4\pi}{Na}, \cdots, \pm\frac{(N-2)\pi}{Na}, \frac{\pi}{a} \quad (N \text{ even})$$

$$q \in \left(-\frac{\pi}{a}, \frac{\pi}{a}\right]$$

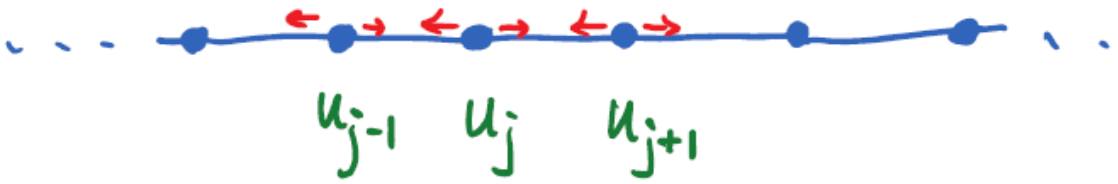
first Brillouin zone (FBZ)



N points in total!

§ 1.1 Classical monoatomic chain

Example: monoatomic chain with nearest-neighbor interactions



Dynamical matrix:

$$D_{jj} = 2C$$

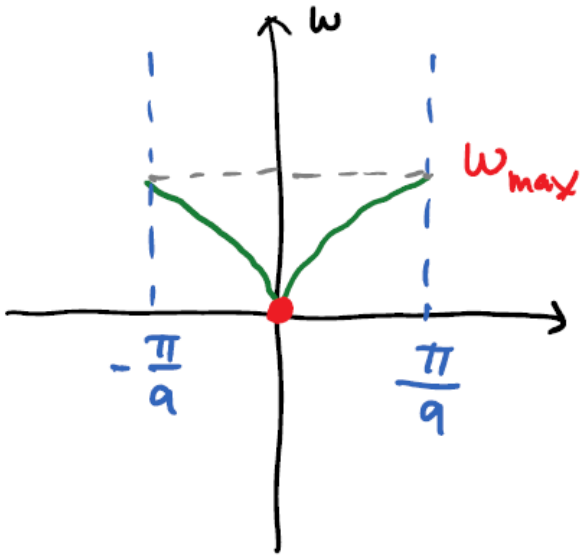
$$D_{j-1,j} = D_{j+1,j} = -C$$

$$V(\{u_j\}) = V_0 + \frac{1}{2} C \sum_{j=1}^{N} (u_j - u_{j+1})^2$$

coupled springs

§ 1.1 Classical monoatomic chain

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



$\omega_{max} = \sqrt{\frac{4C}{M}}$ "cutoff frequency"

§ 1.1 Classical monoatomic chain

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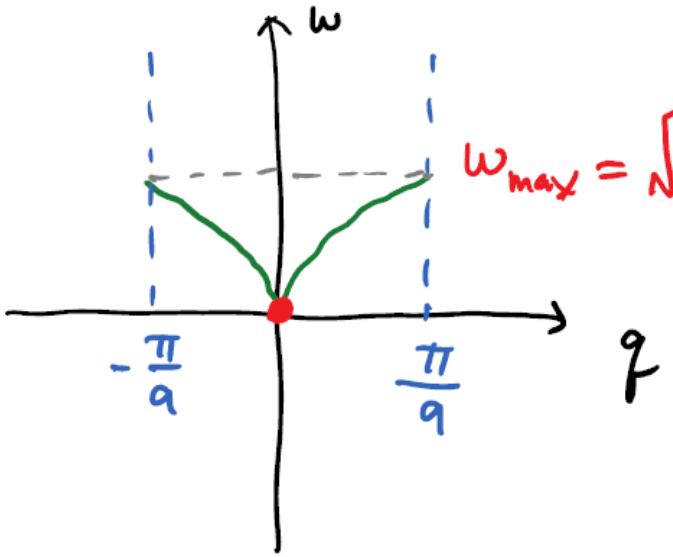

$\omega_{max} = \sqrt{\frac{4C}{M}}$ "cutoff frequency"

Key feature: $\omega_q \to 0$ for $q \to 0$ (long wavelength limit)

$$\boxed{\omega_q \simeq v_s |q|}, \quad v_s = \sqrt{\frac{C}{M}}\, a \text{ (sound velocity)}$$

§ 1.1 Classical monoatomic chain

Interesting interpretations:

- This is perhaps the simplest model for understanding how solids can propagate sound waves.

$$v_s = \sqrt{\frac{C}{M}}\, a \quad \text{(sound velocity)}$$

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- This is perhaps the simplest model for understanding how solids can propagate sound waves.

$$v_s = \sqrt{\frac{c}{M}}\, a \quad \text{(sound velocity)}$$

Estimation of cutoff frequency:

$$\omega_{max} = \sqrt{\frac{4c}{M}} = \frac{2v_s}{a} \approx \frac{10^3\ m/s}{10^{-10}\ m} = 10^{13}\ Hz$$

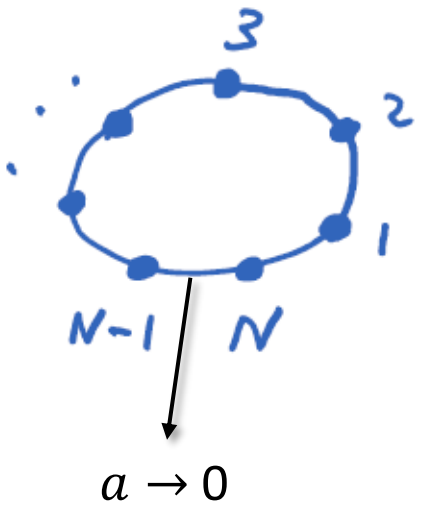
Remark: In the long wavelength limit, the dispersion is always linear if the interaction is short-ranged.

§ 1.1 Classical monoatomic chain

Interesting interpretations:

- Continuum limit describes the vibration of a classical string.

$|q| \to 0$, wavelength $\gg a$



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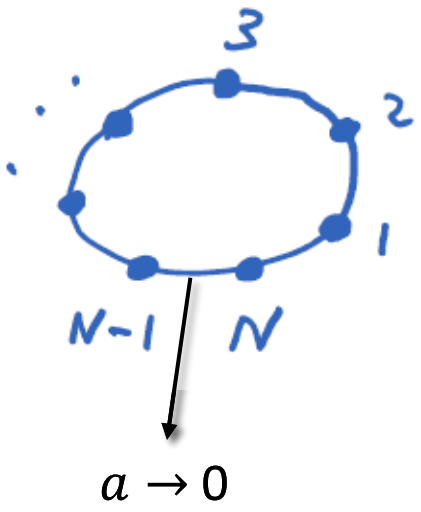
- Continuum limit describes the vibration of a classical string.

$|q| \to 0$, wavelength $\gg a$

$$u_{j+1} - u_j \simeq a\frac{\partial u}{\partial x} + \frac{1}{2}a^2\left(\frac{\partial^2 u}{\partial x^2}\right) + \cdots$$

$$\Rightarrow \quad M\ddot{u} = Ca^2\frac{\partial^2 u}{\partial x^2}$$



elastic wave with velocity $v_s = \sqrt{\frac{C}{M}}\,a$!