SPONTANEOUS SYMMETRY BREAKING

§ 1. Methaphysics

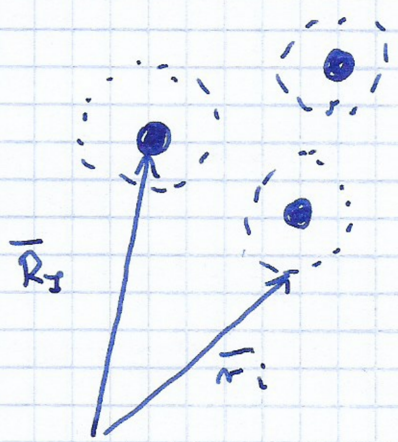
99.99% of everything around us is nonrelativistic

Theory of almost everything (TOAE)

Schrödinger equation

$$\boxed{i\hbar \frac{\partial}{\partial t} \Psi = \hat{\mathcal{H}} \Psi}$$

$$\boxed{\begin{aligned}\hat{\mathcal{H}} = &\sum_{i=1}^{N} -\frac{\hbar^2}{2m} \bar{\nabla}_i^2 + \frac{1}{2} \sum_{i,j=1}^{N} \frac{e^2}{4\pi\varepsilon_0} \frac{1}{|\bar{r}_i - \bar{r}_j|} + \\ &\sum_{I=1}^{M} -\frac{\hbar^2}{2m} \bar{\nabla}_I^2 + \frac{1}{2} \sum_{I,J=1}^{M} \frac{Q^2}{4\pi\varepsilon_0} \frac{1}{|\bar{R}_I - \bar{R}_J|} - \\ &- \sum_{i=1}^{N} \sum_{I=1}^{M} \frac{eQ}{4\pi\varepsilon_0} \frac{1}{|\bar{r}_i - \bar{R}_I|}\end{aligned}}$$



electrons + nuclea

The Hamiltonian of TOAE is

•) translationally invariant,
•) rotationally invariant,
•) time reversible,
•) parity symmetric !

Hamiltonian of TOAE describes plasmas, gases, liquids.

What about solids, crystals, ferromagnets, antiferromagnets, superfluids, superconductors and many others?

In such systems one of the symmetry is absent!

crystals $\longleftrightarrow$ translational symmetry

ferromagnets $\longleftrightarrow$ rotational symmetry

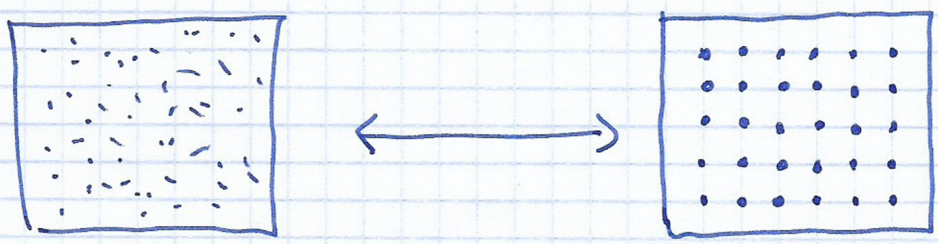
etc.

Common feature $N \simeq 10^{23} \longrightarrow \infty$

When $N \to \infty$ a new quality appears

$\boxed{\text{More is different}}$

P.W. Anderson
Science 1972



§ 2. Spontaneous symmetry breaking

Df.

> Spontaneous symmetry breaking (SSB) is the phenomenon in which a stable state of a system (e.g. the ground state or the thermal equilibrium state) is not symmetric under a symmetry of its Hamiltonian

This is possible if we have an infinitesimal symmetry breaking perturbation h and the system is very large and the limit

$$\boxed{\lim_{h\to 0^+} \lim_{N\to\infty} \langle \hat{O} \rangle \neq 0}$$

on an average of some observable $\hat{O}$ is finite.

Note, that the limit

$$\boxed{\lim_{N\to\infty} \lim_{h\to 0^+} \langle \hat{O} \rangle = 0}$$

Singular limits – these two limiting procedures do not commute.

$$\boxed{\langle \hat{O} \rangle \Big|_{\substack{h\to 0\\ N\to\infty}} = \begin{cases} \text{finite} & \text{– symmetry broken state} \\ \text{zero} & \text{– symmetric state} \end{cases}}$$

$$\boxed{\text{order parameter } \langle \hat{O} \rangle}$$

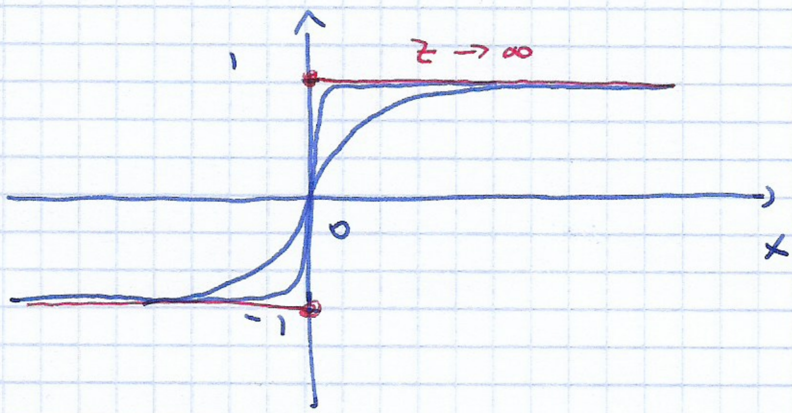
Mathematical example

arctan function

$f(z,x) = \arctan(zx)$

$$\lim_{z\to\infty} \lim_{x\to 0^+} \arctan(zx) = 0$$

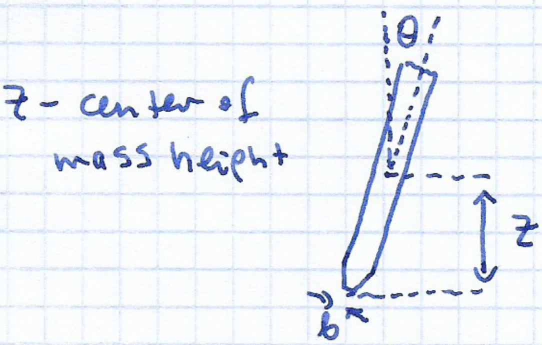
$$\lim_{x\to 0^+} \lim_{z\to\infty} \arctan(zx) = 1$$



When $z \to \infty$ the perturbation (infinitesimally small) of x gives $+1$ or -1. Infinite sensitivity to small perturbation leads to qualitatively different results, which are different from zero.

Mechanical example

pencil balanced on its tip



- not perfectly sharp with a blunt area of diameter b
- not perfectly balanced, dipping by an angle θ - perturbation

symmetric

$$\boxed{\begin{array}{l} \lim_{b\to 0} \lim_{\theta\to 0} z = 1 \\[1em] \lim_{\theta\to 0} \lim_{b\to 0} z = 0 \end{array}}$$

not symmetric

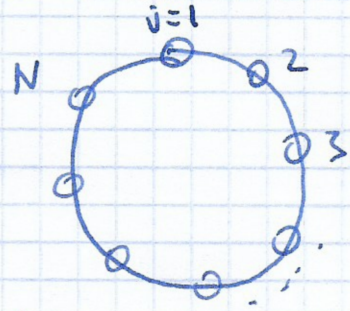
∞ many directions to drop down

§3. Spontaneous symmetry breaking in quantum mechanical model

Am. J. Phys. **75**, 635 (2007)

arxiv: 1909.01820

The harmonic crystal



periodic boundary condition

N atoms on a circle

$j = 1, \dots, N$

$\hat{x}_j$ – position operator

$\hat{p}_j$ – momentum operator

model of harmonic crystal

$$\boxed{\hat{H} = \sum_{j=1}^{N} \frac{\hat{p}_j^2}{2m} + \frac{\varkappa}{2} \sum_{j=1}^{N} \left(\hat{x}_j - \hat{x}_{j+1} \right)^2}$$

bosonic creation and annihilation operators

$$\boxed{\begin{aligned} \hat{p}_j &= i\, C \sqrt{\frac{\hbar}{2}} \left(\hat{b}_j^{+} - \hat{b}_j \right) \\ \hat{x}_j &= \frac{1}{C} \sqrt{\frac{\hbar}{2}} \left(\hat{b}_j^{+} + \hat{b}_j \right) \end{aligned}}$$

$$[\hat{x}_j, \hat{p}_{j'}] = i\hbar\delta_{jj'}$$

$$\updownarrow$$

$$[b_j, b_{j'}^{+}] = \delta_{jj'}$$

$$C^2 = \sqrt{2 m \varkappa}$$

$$\sum_j \frac{\hat{p}_j^2}{2m} = -\frac{\hbar}{2}\frac{1}{2m}\sqrt{2mk}\sum_j (b_j^+ - b_j)(b_j^+ - b_j) =$$

$$= - \frac{\hbar}{4}\sqrt{\frac{2k}{m}}\sum_j \left(b_j^{+2} - b_j^+ b_j - b_j b_j^+ + b_j^2 \right)$$

$$\sum_j \frac{k}{2}(\hat{x}_j - \hat{x}_{j+1})^2 = \frac{k}{2}\frac{\hbar}{2}\frac{1}{\sqrt{2mk}}\sum_j (b_j^+ + b_j - b_{j+1}^+ - b_{j+1})(b_j^+ + b_j - b_{j+1}^+ - b_{j+1}) =$$

$$= \frac{\hbar}{4}\sqrt{\frac{k}{2m}}\sum_j \Big(b_j^{+2} + b_j^+ b_j - b_j^+ b_{j+1}^+ - b_j^+ b_{j+1} +$$

$$+ b_j b_j^+ + b_j^2 - b_j b_{j+1}^+ - b_j b_{j+1} -$$

$$- b_{j+1}^+ b_j^+ - b_{j+1}^+ b_j + b_{j+1}^{+2} + b_{j+1}^+ b_{j+1} -$$

$$- b_{j+1} b_j^+ - b_{j+1} b_j + b_{j+1} b_{j+1}^+ + b_{j+1}^2 \Big) =$$

$$= \frac{\hbar}{4}\sqrt{\frac{k}{2m}}\sum_j \Big(2b_j^{+2} + 2b_j^+ b_j + 2b_j b_j^+ + 2b_j^2 -$$

$$- 2b_j^+ b_{j+1}^+ - 2b_j^+ b_{j+1} - 2b_j b_{j+1}^+ - 2b_j b_{j+1} \Big) =$$

$$= \frac{\hbar}{4}\sqrt{\frac{2k}{m}}\sum_j \Big(b_j^{+2} + b_j^2 + b_j^+ b_j + b_j b_j^+ -$$

$$- (b_j^+ + b_j)(b_{j+1}^+ + b_{j+1}) \Big)$$

$$\boxed{\hat{H} = \frac{\hbar}{4}\sqrt{\frac{2k}{m}}\sum_j \left[2(b_j^+ b_j + b_j b_j^+) - (b_j^+ + b_j)(b_{j+1}^+ + b_{j+1}) \right]},$$

We introduce <u>Fourier transforms:</u>

$$\boxed{\begin{aligned} b_j &= \frac{1}{\sqrt{N}} \sum_k e^{ikaj} \, b_k \\ b_j^+ &= \frac{1}{\sqrt{N}} \sum_k e^{-ikaj} \, b_k^+ \end{aligned}}$$

$$\sum_j b_j^+ b_j = \frac{1}{N} \sum_{kk'} b_k^+ b_{k'} \sum_j e^{i(k-k')aj} = \sum_k b_k^+ b_k$$

$$\sum_j b_j b_j^+ = \sum_k b_k b_k^+$$

$$\sum_j b_j^+ b_{j+1}^+ = \frac{1}{N} \sum_{kk'} b_k^+ b_{k'}^+ \sum_j e^{-ikaj} e^{-ik'a(j+1)} =$$

$$= \sum_{kk'} b_k^+ b_{k'}^+ \frac{1}{N} \sum_j e^{-i(k+k')aj} e^{-ik'a} =$$

$$= \sum_k b_k^+ b_{-k}^+ \, e^{ika}$$

$$\sum_j b_j^+ b_{j+1} = \frac{1}{N} \sum_{kk'} b_k^+ b_{k'} \sum_j e^{-ikaj} e^{ik'a(j+1)} =$$

$$= \sum_{kk'} b_k^+ b_{k'} \frac{1}{N} \sum_j e^{-i(k-k')aj} e^{ik'a} =$$

$$= \sum_k b_k^+ b_k \, e^{ika}$$

$$\sum_j b_j b_{j+1}^+ = \frac{1}{N} \sum_{kk'} b_k b_{k'}^+ \sum_j e^{ikaj} e^{-ik'a(j+1)} =$$

$$= \sum_{kk'} b_k b_{k'}^+ \frac{1}{N} \sum_j e^{i(k-k')aj} e^{-ik'a} =$$

$$= \sum_k b_k b_k^+ \, e^{-ika}$$

$$\sum_j b_j b_{j+1} = \frac{1}{N} \sum_{kk'} b_k b_{k'} \sum_j e^{ikaj} e^{ik'a(j+1)} =$$

$$= \sum_{kk'} b_k b_{k'} \frac{1}{N} \sum_j e^{i(k+k')aj} e^{ik'a} =$$

$$= \sum_k b_k b_{-k} \, e^{-ika}$$

$$\hat{H} = \frac{\hbar}{4}\sqrt{\frac{2K}{m}}\sum_k \Big[2\left(b_k^+ b_k + b_k b_k^+\right) -$$

$$- b_k^+ b_{-k}^+ e^{ika} - b_k b_{-k} e^{-ika} -$$

$$- b_k^+ b_k e^{ika} - b_k b_k^+ e^{-ika} \Big]$$

$$\boxed{\hat{H} = \sqrt{\frac{\hbar^2 K}{2m}} \sum_k \Big[\underbrace{\left(2 - \cos(ka)\right)}_{A_k = A_{-k}} b_k^+ b_k - \underbrace{\frac{\cos(ka)}{2}}_{B_k/2 = B_{-k}/2} \left(b_k^+ b_{-k}^+ + b_k b_{-k}\right) + 1 \Big]}$$

Bogoliubov transformation

$$\boxed{\begin{aligned} b_k^+ &= \cosh(u_k)\,\beta_{-k}^+ - \sinh(u_k)\,\beta_k \\ b_{-k} &= \cosh(u_k)\,\beta_k - \sinh(u_k)\,\beta_{-k}^+ \end{aligned}} \qquad u_k = u_{-k}$$

$$\cosh(2u_k) = \frac{A_k}{\sqrt{A_k^2 - B_k^2}}$$

$$\sinh(2u_k) = \frac{B_k}{\sqrt{A_k^2 - B_k^2}}$$

$$\hat{H} = \sum_k \sqrt{A_k^2 - B_k^2}\left(\beta_k^+ \beta_k + \frac{1}{2}\right) - \frac{1}{2} A_k$$

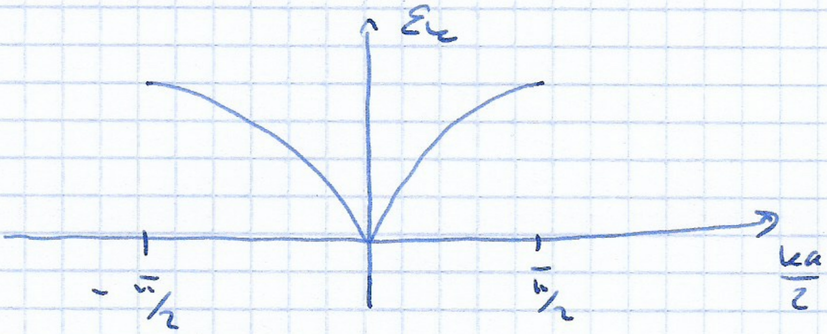
Finally,

$$\sum_k \cos ka = \frac{N}{2\pi}\int_{-\pi}^{\pi} dx \cos x = 0$$

$$\boxed{\hat{H} = 2\hbar\sqrt{\frac{K}{m}} \sum_k \sin\left|\frac{ka}{2}\right| \left[\beta_k^+ \beta_k + \frac{1}{2}\right]}$$

$$\boxed{\varepsilon_k = 2\hbar\sqrt{\frac{K}{m}} \sin\left|\frac{ka}{2}\right|}$$

We have obtained a phonon dispersion



$k = \frac{2\pi}{\lambda}$

wave length

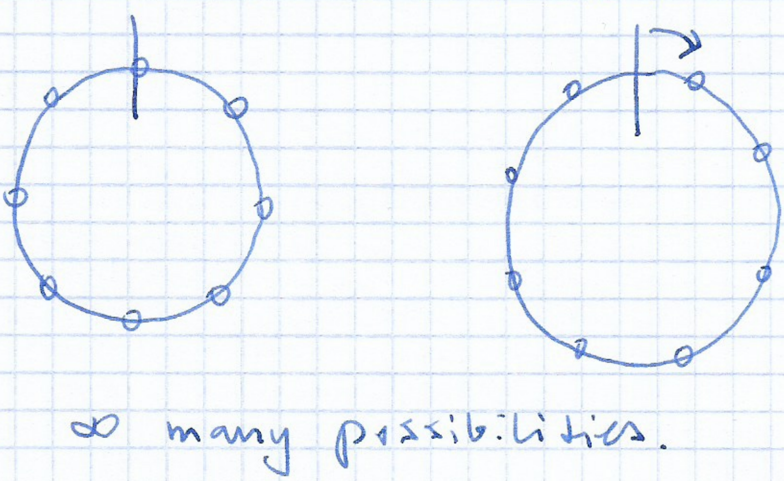
elementary excitations of quantum crystal -
- quasiparticles

At small $ka \ll 1$ $\quad \varepsilon_k \sim |ka|$ — linear

All atoms oscillates around equilibrium positions which are of distance a appart.

They form waves and due to de Broglie hypothesis they correspond to (quantized) particles.

However, where is the origin of this 1d crystal? How is it established?



There are ∞ many possibilities.

The this spectrum and symmetry breaking

When $k \to 0$ we find that $\varepsilon_k \to 0$ but the two parameters in Bogoliubov transformation diverges!

$$\sinh u_k \to \infty$$
$$\cosh u_k \to \infty$$

The $k=0$ limit is not described by the canonical transformation. It must be treated separately from the phonon Hamiltonian.

The $k=0$ part describes the collective dynamics of the crystal as a whole, and therefore such states must be involved in the collective symmetry breaking.

$k=0 \quad \longleftrightarrow \quad \lambda = \infty$ a rigid shift of the whole crystal

$$\hat{H}_{k=0} = \hbar\sqrt{\frac{k}{2m}}\left(b_0^+ b_0 - \frac{1}{2}\left(b_0^+ b_0^+ + b_0 b_0\right) + 1\right) =$$

$$= \hbar\sqrt{\frac{k}{2m}}\left[1 - \frac{1}{2}\left(b_0^+ - b_0\right)^2\right]$$

but $\left(b_0^+ - b_0\right)^2 = -\frac{2}{\hbar\sqrt{2mk}} P_{k=0}^+ P_{k=0}$

where $P_k = \frac{1}{\sqrt{N}}\sum_j e^{ika_j} P_j \quad , \quad P_{k=0} = \frac{1}{\sqrt{N}}\sum_j P_j$

Hence,

$$\boxed{\hat{H}_{k=0} = \frac{\hat{P}_{tot}^2}{2Nm} + \text{const.}}$$

$$\hat{P}_{tot} = \sum_j \hat{p}_j = \sqrt{N}\, p_{k=0}$$

total momentum of the system, center of mass momentum

Since, $[\hat{H}, \hat{P}_{tot}] = 0$ it implies that all eigenstates of the crystal are total momentum eigenstates.

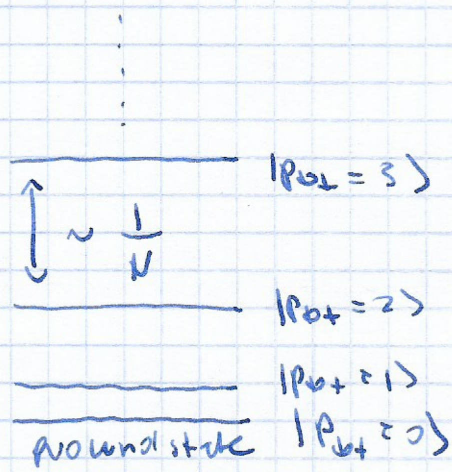
For such states $\Delta P_{tot} = 0$ and due to Heisenberg principle $\Delta X_{CM} = \infty$. The center of mass position is entirely unpredictable.

The total momentum eigenstates wavefunctions are spread out over all of space.

So how the crystal localizes?

The total momentum eigenstates have energy

$$E_{P_{tot}} = \frac{P_{tot}^2}{2mN}$$



They form a bunch of states

energy distance between states scales as $\boxed{\Delta E \sim \frac{1}{N}}$

$$\psi_{P_{tot}=0}(x) = \frac{1}{\sqrt{N}}$$

In the thermodynamic limit $N \to \infty$ all states in the $H_{k=0}$ Hamiltonian are degenerate with the ground state.

Therefore, a wave packet of total momentum states with a well defined center-of-mass position would have the same energy expectation value as the zero-total-momentum eigenstate.

These states do not contribute to the thermodynamics

$$Z_{k=0} = \sum_{p_{tot}} e^{-\beta H_{k=0}} = \int_{-\infty}^{\infty} dp \, e^{-\beta \frac{p^2}{2mN}} = \left\{ \sqrt{\frac{\beta}{2mN}}\, p = x \right\}$$

$$Z_{k=0} \sim \sqrt{N}$$

$$F_{k=0} = -k_B T \ln Z_{k=0} \sim \ln \sqrt{N}$$

$$\frac{F_{k=0}}{F_{k\neq 0}} \sim \frac{\ln N}{N} \xrightarrow[N \to \infty]{} 0$$

Therefore, this part of the spectrum is called the <u>thin spectrum</u> of the quantum crystal.

To see how the thin spectrum conspires to break the symmetry we add a small perturbation

$$\hat{H}_{k=0} = \frac{\hat{P}_{tot}^2}{2mN} + \mu\, \hat{X}_{CM}^2$$

$X_{CM} = \frac{1}{N}\sum_j x_j$ – center of mass position

This is a harmonic oscillator problem

$\omega = \sqrt{\frac{2\mu}{mN}}$, $E_n = \hbar\omega\left(n+\frac{1}{2}\right)$

$$\Psi_0(x) = \left(\frac{2mN\mu}{\pi^2\hbar^2}\right)^{1/8} e^{-\sqrt{\frac{mN\mu}{2\hbar^2}}\,x^2}$$

↑ Gaussian wave packet

$$\sigma^2 = \frac{\hbar}{\sqrt{2mN\mu}}$$

The SSB occurs by appearing two non-commuting limits

$$\lim_{N\to\infty}\lim_{\mu\to 0}|\Psi_0(x)|^2 = \text{const.}$$

$$\lim_{\mu\to 0}\lim_{N\to\infty}|\Psi_0(x)|^2 = \delta(x)$$

The thermodynamic limit is singular!

In both cases $E_0 = \frac{\hbar\omega}{2} = 0$

$$\boxed{\text{In the thermodynamic limit the symmetry broken, localized state of the crystal has the same energy as the exact, plane-wave ground state.}}$$

Estimates: iron (Fe) $m = 9.27\cdot 10^{-26}$ kg, $a = 2.856\cdot 10^{-10}$ m,

$N = 4\cdot 10^{22}$ atoms, $\mu \sim 10^{-14}$ N/m $\to \boxed{\sigma \sim 2\cdot 10^{-12}\ \text{m}}$