1.

## Klasszikus (nemrelativisztikus) mechanika

$v \ll c = 3\ 10^8\ m/s$

$p = m \cdot v = m \cdot \dot{r}$ $\qquad F = \dot{p} = m \cdot \ddot{r}$

## Newton mozgástörvényei = vektormechanika

1. erőmentes térben a test lendülete nem változik
2. a lendületet a testre ható erő változtatja meg.

$$\frac{dmv}{dt} = m \cdot \frac{dv}{dt} = m \cdot a = F$$

3. akció-reakció elve

$$F_{21} = -F_{12}$$

lendületmegmaradás törvénye: $\frac{d}{dt}(p_1 + p_2) = F_{21} + F_{12} = 0$

↓

általánosítva:

$$\frac{d}{dt}\left(\sum_i p_i\right) = 0 \Rightarrow \sum_i p_i = \text{állandó}$$

## Egy rendszer:

tömegközéppontja: $R = \frac{\sum_i m_i \cdot r_i}{\sum_i m_i} = \frac{\sum_i m_i \cdot r_i}{M}$

össztömege: $M = \sum_i m_i$

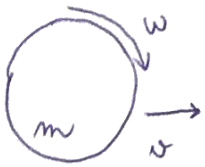
összlendülete: $p = \sum p_i$

sebessége: $V = \frac{dR}{dt}$

perdülete: $L = \sum_i r_i \times p_i = R \times p$

Merev test lendülete és perdülete:

| MENNYISÉGEK | LINEÁRIS MOZGÁS | FORGÓ MOZGÁS | MENNYISÉGEK |
|---|---|---|---|
| távolság | $r$ | $\theta$ | szög |
| sebesség | $v$ | $\omega$ | szögsebesség |
| tömeg | $m$ | $I = m \cdot r^2$ | tehetetlenségi nyomaték |
| lendület | $p$ | $\vec{l} = I \cdot \omega$ | perdület |
| erő | $F (= \dot{p})$ | $M = (\dot{\vec{l}})$ | nyomaték |




kinetikus energia

$$E_{kin} = \frac{1}{2} m v^2 + \frac{1}{2} I \omega^2$$

# Analitikus mechanika

$$F = m\frac{dv}{dt} = m\cdot\ddot{r}(t)$$

Konzervatív erőtér : $F = -\operatorname{grad} U_{pot}(r) = -\nabla U_{pot}$

Szabadon mozgó test : 3 dim $\quad q_1 = x \quad q_2 = y \quad q_3 = z$

$q_1 = r \quad q_2 = \varphi \quad q_3 = \phi$

konfigurációs tér : $q_1, q_2, q_3$

Lagrange függvény : $L = E_{kin} - E_{pot}$

$$L = \frac{1}{2}mv^2 - U_{pot}(r)$$

Hatás : $S[r(t)] = \int_{t_1}^{t_2} L\,dt = \int_{t_1}^{t_2}\left(\frac{1}{2}m\dot{r}^2 - U_{pot}(r)\right)dt$

Legkisebb hatás elve : $\delta S = \delta\int_{t_1}^{t_2} L\,dt = 0$
(Hamilton elv)

Lagrange mozgásegyenletek : (3 másodrendű diff. egyenlet)

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = 0 \qquad i = 1,2,3$$

(Euler-Lagrange egyenlet)

Általános erőhatás : $p_i = \frac{\partial L}{\partial \dot{q}_i} \qquad i = 1,2,3$

Hamilton függvény : $H = \sum_{i=1}^{3} \dot{q}_i p_i - L$

Hamilton-féle kanonikus mozgásegyenletek : (6 elsőrendű diffegy.)

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \qquad \dot{q}_i = \frac{\partial H}{\partial p_i} \qquad i = 1,2,3$$

(2.)

**Gravitáció**: két test között, melyek tömege $m_1, m_2$ mindig vonzóerő hat.

$$F_G = -\gamma \frac{m_1 m_2}{r^2}.$$

$$\gamma = 6.672 \cdot 10^{-11} \ Nm^2 kg^{-2}$$

Speciális eset: gravitáció a Föld felszínén

$$F_G = -\frac{\gamma m_{Föld}}{r^2_{Föld}} \cdot m \cdot e_{Föld} = -m \cdot g \cdot e_{Föld}$$

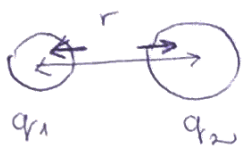
$e_{Föld}$ a Föld középpontja felé mutató egységvektor

$$g \cong 9.81 \frac{N}{kg} \approx 10 \frac{m}{s^2}$$

Elektromos töltéssel rendelkező részecskék

**Coulomb erő**: két töltött test között fellépő vonzás vagy taszítás

$$F_c = \frac{1}{4\pi\varepsilon_0} \cdot \frac{q_1 \cdot q_2}{r^2}$$




$$\varepsilon_0 = 8.85 \cdot 10^{-12} \frac{As}{Vm}$$

$q_1, q_2$ [As] ; r [m] ; F [N]

**Lorentz erő**: elektromágneses erőtérben, mozgó q töltésű testre ható erő.

$$F = q \cdot E + q \cdot (v \times B)$$

F [N]; q [As]; v [m/s]; B [Vs/m²]

B=0 esetén: $F = m \frac{dv}{dt} = q \cdot E$

E=0 esetén: $F = m \frac{dv}{dt} = q(v \times B)$

Relativisztikus esetben, a testek tömege a sebesség növelésével nő.

$v \approx c$

$$mc^2 - m_0c^2 = q(U_2 - U_1)$$

részecske tömegének növelése U feszültséggel:

nyugalmi tömeg $m_0$ k-szorosára növekszik

$$km_0c^2 - m_0c^2 = qU$$

$$U = \frac{(k-1)m_0c^2}{q}$$

tetszőlegesen nagy U gyorsítófeszültség mellett a sebesség:

$$v = c\sqrt{1 - \frac{1}{\left(1 + \frac{qU}{m_0c^2}\right)^2}}$$

tömeg: $$m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}}$$

$D = \varepsilon E + P$
$B = \varepsilon H + M$

## ① Maxwell - egyenletek

→ klasszikus elektrodinamika legfontosabb egyenletei

**I. Maxwell**: áramsűrűség és eltolási áram maga körül mágneses örvényeket gerjeszt

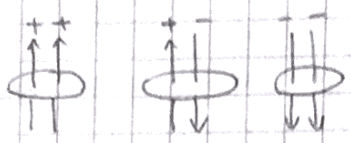
$$\oint_L H \, dl = \int_A \left( J + \frac{\partial D}{\partial t} \right) dA$$

AMPERE TÖRVÉNY

áramsűrűségvektor

$$\nabla \times H = \mathrm{rot}\, H = J + \frac{\partial D}{\partial t}$$

(vektoriális szorzat nablával)

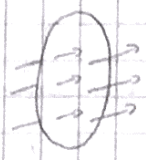


② **II. Maxwell**: időben változó mágneses tér maga körül elektromos térerősség örvényt kelti.

$$\oint_L E \, dl = -\frac{\partial}{\partial t} \boxed{\int_A B \, dA}$$

FAKADAY TÖRVÉNY

FLUXUS



Faraday-féle indukciótörvény:

ha bármely vezető által körülfogott fluxus időben változik, a vezetőben a fluxusváltozással arányos feszültség keletkezik.

$$\nabla \times E = \mathrm{rot}\, E = -\frac{\partial B}{\partial t}$$

③ **III. Maxwell**: mágneses indukcióvektorok nincsenek forrásai

$$\oint_A B \, dA = 0$$

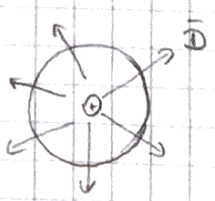
$$\langle \nabla, B \rangle = \mathrm{div}\, B = 0$$

(skalárszorzat nablával)

**IV. Maxwell**: elektromos eltolási vektor "forrásai" az elektromos töltések.

$$\oint_A D \, dA = \sum_i Q_i = \int_V \rho \, dV$$

töltéssűrűség




⇒ felületen áthaladó elektromos eltolási vektorok összessége megegyezik a körülzárt térfogatban levő töltés összességével.

$$\langle \nabla, D \rangle = \mathrm{div}\, D = \rho$$

# (4) ELECTRIC AND MAGNETIC FIELD IN MATTER, POLARIZATION AND MAGNETIZATION MAXWELL V.

Az elektromos teret két vektorral tudjuk leírni:

E: elektromos térerősség vektorok
D: eltolási áram vektorok

$$D = \varepsilon E + P$$

1. eset: vákuum

$$D = \varepsilon_0 E$$

$\varepsilon_0$: vákuum permittivitás

$$\varepsilon_0 \approx 8.854 \cdot 10^{-12} \frac{As}{Vm}$$

2. eset: egyszerű közeg

$$D = \varepsilon E$$

$\varepsilon_{rel}$ = vákuumhoz viszonyított relatív permittivitás

$$\varepsilon = \varepsilon_0 \cdot \varepsilon_{rel}$$

3. eset: általános közeg

$$P(A) = \lim_{\Delta V \to 0} \frac{\Delta p}{\Delta V} \left[\frac{As}{m^2}\right]$$ ← A pontban a polarizációs vektor

P: anyag polarizációs vektora
A: közeg egy pontja
$\Delta V$: pont körüli elemi térfogat
p: $\Delta V$ térfogatban a molekulák dipólusnyomatékának eredője

Teljesül a lineáris anyagegyenlet: $P = \chi \varepsilon_0 E$

$\chi$: dielektromos szusceptibilitás

vákuum: $\chi = 0$
vezető: $\chi = 0$
szigetelő: $\chi > 0$

(4) A mágneses tér két vektorral írható le:

H: mágneses térerősségvektor

B: indukcióvektor

$$B = \mu H + M$$

1. eset: vákuum

$$B = \mu_0 H$$

$\mu_0$: vákuum permeabilitás

$$\mu_0 = 1.256 \cdot 10^{-6} \frac{Vs}{Am}$$

2. eset: egyszerű közeg

$$B = \mu H$$

$$\mu = \mu_0 \cdot \mu_{rel}$$

$\mu_{rel}$: adott közegre jellemző relatív permeabilitás

3. eset: általános közeg

$$M(A) = \lim_{\Delta V \to 0} \frac{\Delta m}{\Delta V} \left[\frac{A}{m}\right]$$

M: mágneses dipólusnyomaték vektor

m: adott $\Delta V$ térfogatban a mágneses dipólusnyomaték eredője

IV. $\nabla \cdot E = 0$

$$A \to B = \nabla \times A; \quad E = -\frac{\partial A}{dt}; \quad \Delta A - \frac{1}{c^2} \cdot \frac{\partial H}{dt^2} = 0$$

# 5. ENERGY AND MOMENTUM OF THE EMAG FIELD.

POYNTING VECTOR.

MAXWELL VI.

Az emag tér energia- és lendület hordozója

## Energiasűrűség egyszerű közegben:

$$w = \frac{1}{2}\langle E, D\rangle + \frac{1}{2}\langle B, H\rangle = \frac{1}{2}\varepsilon\langle E, E\rangle + \frac{1}{2}\mu\langle H, H\rangle \quad \left[\frac{Ws}{m^3}\right]$$

Az összenergia adott térfogatban megegyezik a mágneses és elektromos energiák összegével → energiasűrűség térfogati integrálja

$$\int_V w\, dV = \int_V \frac{1}{2}\varepsilon\langle E, E\rangle + \frac{1}{2}\mu\langle H, H\rangle\, dV$$

## Véges térfogatú emag tér energiája

emag energia megváltozásának okai:

- generátorok energiát szolgáltatnak
- energia egy része hővé alakul
- az energia egy része a zárt térfogat határoló felületen át sugárzással távozik

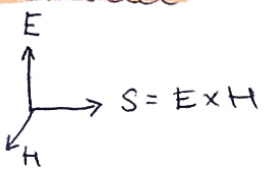
## Emag energia megmaradásának tétele:

$$\underbrace{\int_V \langle E_{gen}, J\rangle\, dV}_{} = \underbrace{\frac{\partial}{\partial t}\int_V \left(\frac{1}{2}\mu\langle H, H\rangle + \frac{1}{2}\varepsilon\langle E, E\rangle\right) dV}_{} + \underbrace{\int_V \frac{\langle J, J\rangle}{\sigma}\, dV}_{} + \underbrace{\oint_A E\times H\, dA}_{}$$

V-beli generátor által termelt teljesítmény = V-ben tárolt egységnyi idő alatti energianövekedés + V-ben hővé alakuló teljesítmény + A felületen V-ből kilépő sugárzó telj.

## Térben áramló emag teljesítmény → lendület

$$S = E\times H \quad \left[\frac{W}{m^2}\right] = \left[\frac{VA}{m^2}\right]$$




* dielektrikum: elektromosan szigetelő anyag

S: Poynting-vektor → sugárzást leíró vektor, mely merőleges az elektromos és mágneses térerősségre

E és / vagy H ≠ 0 → energia van a térben

S = E × H ≠ 0 → energia áramlik még stacionárius esetben is

OK: az EMAG energia mindig a dielektrikumban terjed.

## 6. STATIC AND STATIONARY APPROXIMATIONS OF THE EMAG COULOMB AND BIOT SAVART LAWS.

### Sztatikus elektromos térre vonatkozó inverz-probléma

Feltevések: → egyszerű közeg: $D = \varepsilon E$

→ IV. Maxwell egyenlet: $\langle \nabla, D \rangle = \rho$

$\rho$ ↓ töltéssűrűség

1.) $\langle \nabla, D \rangle = \rho$

$\langle \nabla, E \rangle = \frac{\rho}{\varepsilon}$

2.)* $E = -\nabla U$ (elektromos tér a skalárpotenciál ($U$) negatív gradienseként előáll)

$-\langle \nabla, \nabla U \rangle = \frac{\rho}{\varepsilon}$

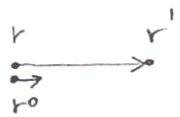
3.) $\nabla^2 = \Delta$

$\Delta U(r) = -\frac{\rho(r)}{\varepsilon}$ POISSON-EGYENLET (differenciál egyenlet)

4.) $U(r) = \frac{1}{4\pi\varepsilon} \int_V \frac{\rho(r')}{|r-r'|} dV'$

| | | |
|---|---|---|
| töltés ($\rho$) | → skalárpotenciál ($U$) | → E |

5.) $E(r) = -\text{grad}\, U(r) = \frac{1}{4\pi\varepsilon} \int_V \frac{\rho(r') r^0}{r^2} dV'$




$r^0$: r helyvektorú pontból az r' helyvektorú pont felé mutató egységnyi hosszú vektor

$r^2$: két pont távolságának négyzete

### Stacionárius mágneses tér inverz problémája

Kiindulás: → $D = \varepsilon E$

→ $B = \mu H$

→ I. Maxwell egyenlet: $\nabla \times H = J$

1.)* $B = \nabla \times A$ (mágneses tér a vektorpotenciál ($A$) rotációjával áll elő)

2.) $\nabla \times H = J$

$\nabla \times B = \mu J$

$\Rightarrow \quad \nabla \times (\nabla \times A) = \mu J$

3.) $\nabla \times \nabla \times A = \underbrace{\nabla \langle \nabla, A \rangle}_{0} - \Delta A$

$\nabla \times (\nabla \times A) = -\Delta A = \mu J$

4.) $A(r) = \frac{\mu}{4\pi} \int_V \frac{J(r')}{r} dV'$

| |
|---|
| áramsűrűség $(J)$ → vektorpotenciál $(A)$ → B |

5.) $B(r) = \nabla \times A = \frac{\mu}{4\pi} \nabla \times \int_V \frac{J(r')}{\underbrace{|r - r'|}_{r}} dV'$

**Coulomb törvény:** két pont közötti elektromos kölcsönhatásból származó erő

1.) pontszerű töltés:

$Q = \int_V \rho \, dV$

2.) pontszerű töltés erőtere:

$E(r) = \frac{1}{4\pi\epsilon} \int_V \frac{\rho(r') r^0}{r^2} dV'$

3.) q töltésre ható erő, Coulomb törvény

$F = q \cdot E = \frac{q \cdot Q}{4\pi\epsilon r^2} = k \cdot \frac{q \cdot Q}{r^2}$

$k = \frac{1}{4\pi\epsilon}$

**Biót-Savart törvény:** áramvezető által keltett mágneses teret egy P pontban meg tudjuk adni.

$B(r) = \frac{\mu}{4\pi} \nabla \times \int_V \frac{J(r)}{\underbrace{|r - r'|}_{r}} \underbrace{dA\,dl} = \frac{\mu I}{4\pi} \int_L \nabla \times \frac{1}{r} dl = \frac{\mu I}{4\pi} \int_L \frac{dl \times r^0}{r^2}$

## II. Kirchoff törvény

hurokáramok törvénye, azaz zárt hurok mentén a feszültségesések és emelkedések összege zérus. $\sum_i U_i = 0$

Kiindulás: → II. Maxwell egyenlet

1.) II. Maxwell egy: $\nabla \times E = 0$

2.) Stokes tételt felhasználva:

* $\int_A \nabla \times E \, dA = \oint_L E \, dl = 0$

Differenciális Ohm-törvény

* $J = \sigma (E + E_{gen})$

$E = \frac{J}{\sigma} - E_{gen}$

$\Rightarrow \oint_L E \, dl = \oint_L \left( \frac{J}{\sigma} - E_{gen} \right) dl = 0$

3.) 1-gyel szorzás $\left( \cdot \frac{A}{A} \right)$

$\oint_L \left( \frac{JA}{A\sigma} - E_{gen} \right) dl = I \cdot \oint_L \frac{1}{A\sigma} \, dl - \oint_L E_{gen} \, dl = 0$

4.) $\sum_k I_k R_{ik} - \sum_k U_{gen_k} = 0$

$\frac{1}{A\sigma}$ ellenállás (R) dimenziójú

k. indexű generátor által szolgáltatott villamos térerősség vonalmenti integrálja megegyezik a hálózatba jelöltetett külső potenciál értékével

$\nabla \times E = 0$

Stokes

$\int_A \nabla \times E \, dA = \oint_L E \, dl = 0$

$J = \sigma (E + E_{gen})$

$E = \frac{J}{\sigma} - E_{gen}$

$\oint_L E \, dl = \oint_L \frac{J}{\sigma} - E_{gen} \, dl = 0$

$\oint_L \left( \frac{JA}{\sigma A} - E_{gen} \right) dl$

$I \cdot \oint_L \frac{1}{A\sigma} - \oint_L E_{gen} \, dl$

$I_k R_{ik} - U_{gen}$

# (7.) FROM MAXWELL'S EQUATIONS TO KIRCHOFF'S LAWS (STATIONARY APPROXIMATION)

A stacionárius (egyenáramú) áramkörökben igaz Kirchoff törvényeket levezethetjük a Maxwell egyenletekből is.

I. Kirchoff-törvény:

töltésmegmaradás elve, azaz a befolyó és kifolyó áramok előjeles összege zérus.

$$\sum_k I_k = 0$$

Kiindulás: → I. Maxwell : $\nabla \times H = J + \frac{\partial D}{\partial t}$

→ IV. Maxwell : $\langle \nabla, D \rangle = \rho$

1.) ha az I. Maxwell egyenlet divergenciáját képezzük, 0-t kapunk

$$\langle \nabla, \nabla \times H \rangle = \langle \nabla, J \rangle + \langle \nabla, \frac{\partial D}{\partial t} \rangle = 0$$

$\rho$

2.) $\langle \nabla, D \rangle = \rho$ behelyettesítés

$$\langle \nabla, J \rangle + \frac{\partial \rho}{\partial t} = \langle \nabla, J \rangle = 0$$

↓

a töltéssűrűség nem változik az stacionárius körülmények mellett

3.) Gauss-Osztrogradszkij tétel felhasználása

$$* \oint_A F \, dA = \int_V \operatorname{div} F \, dV$$

$$\int_V \langle \nabla, J \rangle \, dV = \oint_A J \, dA = \sum_k I_k = 0$$

5. Electromagnetic field in an empty cavity. Vector potential as state variable.
Cavity modes. Lagrangian of a cavity mode. Complete orthonormal set.

6/1

$$E(r,t) = -\frac{\partial A(r,t)}{\partial t}$$
$$B(r,t) = \nabla \times A(r,t)$$

classical EMAG in vacuum

SEPARATION METHOD

$$A(r,t) = f(t)\cdot A(r) \Longleftarrow \Delta A(r,t) - \frac{1}{c^2}\frac{\partial^2 A(r,t)}{\partial t^2} = 0$$

wave equation for vector potential

Cavity modes => normalized solutions

$A_1(r),\ A_2(r), \dots, A_n(r), \dots$

Cavity modes form a complete orthonormal set

$$A(r,t) = \sum_n f_n(t)\cdot A_n(r)$$

Electric and magnetic field of a mode

$$E_k(r,t) = \frac{d f_k(t)}{dt}\cdot A_k(r) \qquad B_k(r,t) = f_k(t)\cdot \nabla\times A_k(r)$$

Electric and magnetic energies stored in a mode

$$E_{Ek} = \int_V \left(\frac{1}{2}\varepsilon_0 E_k(r,t)^2\right) dV \qquad E_{Mk} = \int_V \left(\frac{1}{2\mu_0}\cdot B_k(r,t)^2\right) dV$$

$$= \frac{1}{2}\varepsilon_0 \cdot \left[\frac{d f_n(t)}{dt}\right]^2 \qquad = \frac{k_n^2}{2\mu_0}\cdot f_n(t)^2$$

Lagrangian of a cavity mode

$$L_k = E_{Ek} - E_{Mk} = \frac{1}{2}\varepsilon_0 \left[\frac{d f_k}{dt}\right]^2 - \frac{k_n^2}{2\mu_0}\cdot f_k^2$$

Time-domain dynamics:

$$\frac{d^2 f_n(t)}{dt^2} = -\frac{k_n^2}{\varepsilon_0\mu_0}\cdot f_n(t) = -\omega_n^2\cdot f_n(t)$$

Vector potential as state variable

Maxwell Equations in vacuum

I. $\nabla\times H = \frac{\partial D}{\partial t} = \varepsilon_0\cdot\frac{\partial E}{\partial t} \rightarrow E = \frac{\partial A}{\partial t}$

vektorpotenciál

$$\frac{1}{\mu_0}\cdot\nabla\times\underbrace{\nabla\times A}_{B} = \varepsilon_0\cdot\frac{\partial^2 A}{\partial t^2}$$

H

II. $\nabla\times E = -\frac{\partial B}{\partial t} \rightarrow \nabla\times E = -\nabla\times\frac{\partial A}{\partial t}$

$B = \nabla\times A$

$$\nabla\times\left(E + \frac{\partial A}{\partial t}\right) = 0 \leftarrow \nabla\times E + \nabla\times\frac{\partial A}{\partial t} = 0$$

$$E + \frac{\partial A}{\partial t} = -\nabla\cdot\varphi$$

skalárpotenciál

III. $\nabla\cdot B = 0 \rightarrow B = \nabla\times A$, $\nabla\cdot A = 0$

IV. $\nabla\cdot E = 0$

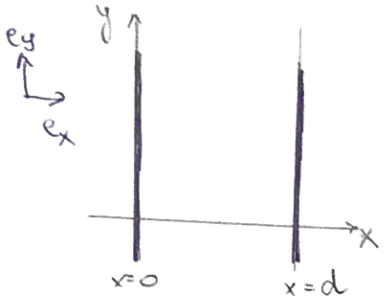
$$A \rightarrow B = \nabla\times A;\ E = -\frac{\partial A}{dt};\ \Delta A - \frac{1}{c^2}\cdot\frac{\partial^2 A}{dt^2} = 0$$

div $\quad f_x + f_y + f_z \quad + p$

$v = (x, y, z)$

# The electromagnetic waves in a one dimensional cavity

waves between two parallel mirrors




The spatial eigenvalue problem

$$\Delta A_n(r) = -k_n^2 \cdot A_n(r)$$

$$A_n(r) = A_n(x) \cdot \overset{1}{e_y} \rightarrow \text{hely felbontása x,y tengelyekre}$$

MÁSODRENDŰ PARCIÁLIS DE

$$u(x,y) = X'' \cdot Y + Y'' X$$

$$\frac{X''}{X} = -\frac{Y''}{Y} := \lambda$$

szeparábilis módszerrel

$$\lambda = -k_n^2$$

$$X'' = \lambda \cdot X \Rightarrow \frac{d^2 A_n(x)}{dx^2} = -k_n^2 \cdot A_n(x)$$

$$\Delta A_n(r) = -k_n^2 \cdot A_n(r)$$

**Általános megoldás**

$$A_n(x) = c_1 \cdot \sin(k_n x) + c_2 \cdot \cos(k_n x)$$

$$E_n(r,t) = \frac{\partial A(r,t)}{\partial t} = \frac{d f_n(t) \cdot A(r)}{dt} = \frac{d f_n(t)}{dt} \cdot A(r)$$

kezdeti feltételek: $A_n(0) = A_n(d) = 0$

$$A_k(0) = 0 = c_1 \cdot \sin(k_n x) + \underbrace{c_2 \cdot \cos(k_n x)}_{0}$$

$$A_k(d) = 0 = c_1 \cdot \sin(k_n x)$$

$$\Rightarrow k_n d = n\pi \Rightarrow k_n = \frac{n\pi}{d} \quad n = 1, 2 \ldots$$

$$A_{kn}(x) = c_1 \cdot \sin\left(\frac{n\pi}{d} \cdot x\right)$$

$$\int_0^d A_n^2(x)\,dx = \int_0^d c_1^2 \cdot \sin^2\left(\frac{n\pi}{d} x\right) dx = 1$$

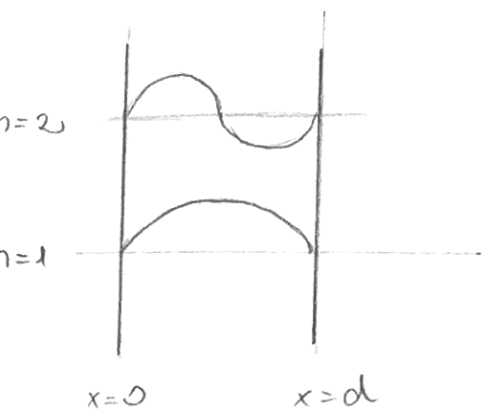
$$A_n(x) = \sqrt{\frac{2}{d}} \cdot \sin\left(\frac{n\pi}{d} x\right) \quad n = 1, 2 \ldots$$

---

$$E_n(x,t) = -\frac{d f_n(t)}{dt} \cdot e_y \cdot \sqrt{\frac{2}{d}} \cdot \sin\left(\frac{n\pi}{d} \cdot x\right)$$

$$E_n(x,t) = \underbrace{\boxed{F_n \cdot \sin(\omega_n t + \phi_n)}}_{\text{időfüggő}} \cdot \underbrace{\boxed{e_y \cdot \sqrt{\frac{2}{d}} \cdot \sin\left(\frac{n\pi}{d} x\right)}}_{\text{helyfüggő}}$$

$$-\frac{d f_n(t)}{dt} = F_n \cdot \sin(\omega_n t + \phi_n)$$



14. Representation of quantum objects by kets, bras, brackets and operators in a Hilbert space.
Algebra in a Hilbert space.
Inner and outer products.

6/4

In quantum mechanics, bra-ket notation is a standard notation for describing quantum states. Paul Dirac in the late 1920's introduced this short-hand notation, which helped to generalize the state representation.

The state wave functions are described by "ket"-s.

$$\psi(q_1, q_2, \dots q_f, t) \Longleftrightarrow |\psi\rangle \quad \text{KET}$$

The complex conjugate of the wave function is described by "bra".

$$\psi^*(q_1, q_2, \dots, q_f, t) \Longleftrightarrow \langle\psi| \quad \text{BRA}$$

The scalar product is described by "bracket".

$$\int_V \psi_a^* \psi_b \, dV \Longleftrightarrow \langle\psi_a|\psi_b\rangle$$

The expectation value

$$\langle L\rangle = \int_V \psi^* \hat{L} \psi \, dV \Longleftrightarrow \langle\psi^*|\hat{L}|\psi\rangle$$

The eigen functions are: $|1\rangle, |2\rangle, \dots, |n\rangle$

## KET $|\alpha\rangle$

In quantum physics a physical state is represented by a state vector, called "ket", which contains the complete information about the physical state. Hilbert space is the complex vector space, where the ket is represented

The dimension of the vector space depends on the physical system.

Algebra of "ket"

$|a\rangle, |b\rangle \in \mathcal{H}$

$|a\rangle + |b\rangle = |c\rangle \in \mathcal{H}$

$\lambda|a\rangle = |a\rangle\lambda \in \mathcal{H}$ $\quad \lambda$: complex number

null ket: $\lambda|a\rangle$ if $\lambda = 0$

1

$|a\rangle$ and $\lambda|a\rangle$ with $\lambda \neq 0$ represent the same physical state.
Only the direction in the vector space is important!

## BRA : $\langle b|$

KET : $|a\rangle$
BRA : $\langle a|$ } $\overset{\text{duality}}{|a\rangle \Longleftrightarrow \langle a|}$ for $\forall |a\rangle$

The "bra"-space is the dual vector space of the "ket"-space.

Rules of duality:

$|a\rangle \Longleftrightarrow \langle a|$

$|a\rangle + |b\rangle \Longleftrightarrow \langle a| + \langle b|$

$c_a \cdot |a\rangle + c_b \cdot |b\rangle \Longleftrightarrow c_a^* \cdot \langle a| + c_b^* \cdot \langle b|$

eigenkets and their dual eigenbras : $\{|a^{(n)}\rangle\} \Longleftrightarrow \{\langle a^{(n)}|\}$

$\{|n\rangle\} \Longleftrightarrow \{\langle n|\}$

## BRACKET : $\langle b|a\rangle$

The scalar product of a "bra" and a "ket" is the "bracket".

$\langle b|a\rangle$ = number (in general complex) $\qquad \langle b|a\rangle = \langle a|b\rangle^*$ complex conjugate

$\langle b|a\rangle$ bracket is the INNER PRODUCT of $\langle b|$ "bra" and $|a\rangle$ "ket".

$\langle a|a\rangle$ = real number; $\quad \langle a|a\rangle \geq 0$

if $\langle a|a\rangle = 0 \rightarrow |a\rangle$ is a null ket

to kets are orthogonal $\quad |a\rangle \perp |b\rangle$

if $\langle a|b\rangle = 0$ inner product

normalized ket

$$|\bar{a}\rangle = \frac{1}{\sqrt{\langle a|a\rangle}} \cdot |a\rangle$$

$\langle \bar{a}|\bar{a}\rangle = 1$

## OPERATORS $\hat{X}, \hat{Y}, \hat{Z}$

The observable is represented by a linear operator.

Real world → strong measurement → get the eigenvalues of the operator → set of countably infinite elements → depending on the state (ket) get the probabilities of the elements

$\hat{A}(|a\rangle) = \hat{A}|a\rangle \in \mathcal{H}$ operator acts on the ket from left → → maps a ket on a ket

$(\langle b|)\hat{A} = \langle b|\hat{A} \in \mathcal{H}$ operator acts on the bra from right → → maps a bra on a bra

$\hat{X} = |a\rangle\langle b|$ the operator is the OUTER PRODUCT of $|a\rangle$ ket and $\langle b|$ bra

### Algebra of the operator

$\hat{X} = \hat{Y}$ if $\hat{X}|a\rangle = \hat{Y}|a\rangle$ for $\forall |a\rangle$

if $\hat{X}|a\rangle = 0$ for $\forall |a\rangle$ $\Rightarrow$ $\hat{X}$ null operator

### Summation of operator:

$\hat{X} + \hat{Y} = \hat{Y} + \hat{X}$ commutative

$\hat{X} + (\hat{Y} + \hat{Z}) = (\hat{X} + \hat{Y}) + \hat{Z}$ associative

### Linear operator:

$\hat{X}(c_a|a\rangle + c_b|b\rangle) = c_a \cdot \hat{X}|a\rangle + c_b \cdot \hat{X}|b\rangle$

### Products of operator in general:

$\hat{X}\hat{Y} \neq \hat{Y}\hat{X}$ <u>NOT</u> commutative, the order of operators is important

$\hat{X}(\hat{Y}\hat{Z}) = (\hat{X}\hat{Y})\hat{Z} = \hat{X}\hat{Y}\hat{Z}$ associative

### 2 operator acting on a ket/bra:

$\hat{X}(\hat{Y}|a\rangle) = (\hat{X}\hat{Y})|a\rangle = \hat{X}\hat{Y}|a\rangle$ (KET)

$\langle b|\hat{X}\hat{Y} = \langle b|\hat{X}(\hat{Y}) = (\langle b|\hat{X})\hat{Y}$ (BRA)

### $\langle a|\hat{X}|b\rangle$ notation:

$\underbrace{\langle a|}_{\text{bra}} \cdot \underbrace{(\hat{X}|b\rangle)}_{\text{ket}} \equiv \underbrace{(\langle a|\hat{X})}_{\text{bra}} \cdot \underbrace{|b\rangle}_{\text{ket}} \equiv \langle a|\hat{X}|b\rangle$

bra × ket = bra × ket

## Legal and illegal products between kets, bras and operators

6/4

$$\underbrace{\underbrace{(|a\rangle\langle b|)}_{\text{matrix}} \times \underbrace{|c\rangle}_{\text{ket}}}_{\text{ket}} = \underbrace{\underbrace{|a\rangle}_{\text{ket}} \times \underbrace{(\langle b|c\rangle)}_{\text{complex number}}}_{\text{ket}} \quad ✓$$

But: $(\langle b|c\rangle)\cdot|a\rangle \neq \langle b|\cdot(\cancel{|c\rangle|a\rangle})$

$$\underbrace{|c\rangle}_{\text{ket}} \times \underbrace{\cdot|a\rangle}_{\text{ket}} \quad ↯$$

15. Eigenvalues, eigenvectors in a Hilbert space.

Linear and self-adjoint operators → SEE TOPIC 16.

Orthonormal set of eigenvectors. → SEE TOPIC 16.

The completeness theorem. * → TOPIC 16.

The observable is represented by a linear operator : $\hat{A}\cdot(|a\rangle) = \hat{A}|a\rangle \in \mathcal{H}$

In general $\hat{A}|a\rangle \neq c\cdot|a\rangle$ but there are such kets

$$\hat{A}|a^{(n)}\rangle = a^{(n)}\cdot|a^{(n)}\rangle$$

$$\hat{A}|a^{(n)}\rangle = a_{(n)}\cdot|n\rangle$$

$a^{(1)}, a^{(2)}, \dots, a^{(n)}$ eigenvalues of operator $\hat{A}$

$|a^{(1)}\rangle, |a^{(2)}\rangle, \dots, |a^{(n)}\rangle$ eigenkets

$|1\rangle, |2\rangle, \dots, |n\rangle$ eigenkets

In an N-dimensional vektor space every ket can be expressed as

$|a\rangle = \sum_n c_n\cdot|a^{(n)}\rangle$ linear combination of eigenkets

$$|a\rangle = \sum_n c_n\cdot|n\rangle$$

In quantum physics the observables can be represented by linear self-adjoint operators.

Lemma I.

Eigenvalues of self-adjoint operators are real numbers.

The eigenkets are orthogonal to each other.

$$\hat{A}|n\rangle = a^{(n)}\cdot|n\rangle$$

↳ real number

$|1\rangle, |2\rangle, \dots, |n\rangle$ eigenkets

$$\langle i|j\rangle = \delta_{ij} \begin{cases} 1 & \text{if } i=j \\ 0 & \text{if } i\neq j \end{cases}$$ orthonormality

Lemma II.

Eigenkets constitute a complete orthonormal basis.

$$|a\rangle = \sum_n c_n\cdot|n\rangle \qquad c_n = \langle n|a\rangle$$

if $|a\rangle$ is normalized, then $\sum_n |c_n|^2 = \sum_n |\langle n|a\rangle|^2 = 1$

16. Operators in a Hilbert space. 6/5

Zero, unit, adjoint, self-adjoint and projection operators.

Properties of a self adjoint operator. Basis in a Hilbert space.

Commutator of two operators.

**OPERATORS $\hat{X}, \hat{Y}, \hat{Z}$** → see also topic 14!

$\hat{X}$ is a zero/null operator

if $\hat{X}|a\rangle = 0$ for $\forall |a\rangle$

$\hat{X}$ is a linear operator

if $\hat{X}(c_a|a\rangle + c_b|b\rangle) = c_a \cdot \hat{X}|a\rangle + c_b \cdot \hat{X}|b\rangle$

$\hat{X}^\dagger$ is an adjoint operator of $\hat{X}$

if $\hat{X}|a\rangle$ and $\langle a|X^\dagger$ are dual

$\forall \hat{X}|a\rangle$ - hoz tartozik $\langle a|X^\dagger$ párt

$\hat{X}$ ketet $\leftrightarrow$ $\hat{X}^\dagger$ bratra

$(\hat{X}\hat{Y})^\dagger = \hat{Y}^\dagger \cdot \hat{X}^\dagger$ $\qquad \hat{X} = |a\rangle\langle b| \rightarrow \hat{X}^\dagger = |b\rangle\langle a|$

If $\hat{X} = \hat{X}^\dagger$, $\hat{X}$ operator is equal to its $\hat{X}^\dagger$ adjoint operator, then

$\hat{X}$ is a self-adjoint operator.

$\langle b|\hat{X}|a\rangle = \langle b| \cdot (\hat{X}|a\rangle) = [(\langle a|\hat{X}^\dagger) \cdot |b\rangle]^* = \langle a|X^\dagger|b\rangle^*$

In quantum physics the mathematical representation of observables are linear self-adjoint operators.

**Lemma I.**

Eigenvalues of a self-adjoint operator are real numbers

The eigenkets belonging to different eigenvalues are orthogonal

$\hat{A}|n\rangle = a^{(n)} \cdot |n\rangle$ $\qquad a^{(1)}, a^{(2)}, \dots, a^{(n)}$ eigenvalues of $\hat{A}$

$|1\rangle, |2\rangle, \dots, |n\rangle$ eigenkets of the eigenvalues

$$\langle i|j\rangle = \delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$ orthonormality

**Lemma II.**

Eigenkets constitute a complete orthonormal basis.

$|a\rangle = \sum_n c^{(n)} |n\rangle$ $\qquad c^{(n)} = \langle n|a\rangle$ ← PROBABILITY OF THIS STATE

minden ket előáll az eigenketek lineáris kombinációjával

$|a\rangle = \sum_n |n\rangle\langle n|a\rangle$ $\qquad \sum_n |n\rangle\langle n| = \hat{1}$ is the unit operator

$$\langle a|a\rangle = \langle a| \underbrace{\sum_n |n\rangle\langle n|}_{1} \rangle \cdot |a\rangle = \sum_n |\langle n|a\rangle|^2$$

if $|a\rangle$ is normalized, then $\sum_n |c_n|^2 = \sum_n |\langle n|a\rangle|^2 = 1$

sum of probabilities must be 1

**Projection operator**: $\hat{\Lambda}_n$

$$\hat{\Lambda}_n = |n\rangle\langle n|$$

$$\hat{\Lambda}_{a^{(n)}} \cdot |a\rangle = |n\rangle \underbrace{\langle n|a\rangle}_{c_n} = c_n \cdot |n\rangle$$

$a^{(n)}$ sajátértékhez tartozó $|n\rangle$ sajátvektor

$$\sum_n \hat{\Lambda}_n = \hat{1} \qquad \text{completeness}$$

**Commutator of two operators** $[\hat{A}, \hat{B}]$

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = \begin{cases} 0 & \text{if } \hat{A} \text{ and } \hat{B} \text{ commute} \\ \text{else} & \text{if } \hat{A} \text{ and } \hat{B} \text{ don't commute} \end{cases}$$

If ~~and~~ $\hat{A}$ and $\hat{B}$ commute, then their order can be exchanged.

17. Matrix representation of kets, bras and operators in Hilbert space.

X

6/6

In quantum physics the representation of observables are linear self-adjoint operators.

Lemma 2.: eigenkets constitute a complete orthonormal basis

$|a\rangle = \sum_n c_n \cdot |n\rangle \qquad c_n = \langle n|a\rangle$

$|a\rangle = \underbrace{\sum_n |n\rangle\langle n|}_{\hat{1}} a\rangle \qquad \sum_n |n\rangle\langle n| = \hat{1}$ unit operator → sends each vector to itself.

because of orthonormality

$\langle i|j\rangle = \delta_{ij} \begin{cases} 1 & \text{if } i=j \\ 0 & \text{if } i \neq j \end{cases}$

If N is the dim of the space of the kets, the representation of operator $\hat{X}$:

$$\hat{X} = \hat{X} \rightarrow \hat{X} = \underbrace{\left(\sum_{n=1}^{N} |n\rangle\langle n|\right)}_{1} \cdot \hat{X} \cdot \underbrace{\left(\sum_{m=1}^{N} |m\rangle\langle m|\right)}_{1} =$$

$$= \sum_{m=1}^{N}\sum_{n=1}^{N} |m\rangle \boxed{\langle m|\hat{X}|n\rangle} \langle n|$$

row vector — $N^2$ number — column vector

mátrixban számok!

$$\hat{X} = \begin{bmatrix} \langle 1|\hat{X}|1\rangle & \langle 1|\hat{X}|2\rangle & \dots & \langle 1|\hat{X}|N\rangle \\ \langle 2|\hat{X}|1\rangle & \langle 2|\hat{X}|2\rangle & \dots & \langle 2|\hat{X}|N \\ \vdots & \vdots & & \vdots \\ \langle N|\hat{X}|1\rangle & \langle N|\hat{X}|2\rangle & \dots & \langle N|\hat{X}|N\rangle \end{bmatrix}$$

$|a\rangle = \sum_n c_n \cdot |n\rangle = \sum_n \langle n|a\rangle |n\rangle = \underbrace{\sum_n |n\rangle\langle n|}_{1} a\rangle$

$|b\rangle = \hat{X}|a\rangle$

$|a\rangle = \sum_n |n\rangle \boxed{\langle n|a\rangle}$ valószínüségek

egységvektorokra bontás bázisszal való felírása

$|b\rangle = \sum_n |n\rangle \boxed{\langle n|b\rangle}$

$$|a\rangle = \begin{bmatrix} \langle 1|a\rangle \\ \langle 2|a\rangle \\ \langle 3|a\rangle \\ \vdots \\ \langle N|a\rangle \end{bmatrix} \qquad |b\rangle = \begin{bmatrix} \langle 1|b\rangle \\ \langle 2|b\rangle \\ \vdots \\ \langle N|b\rangle \end{bmatrix}$$

számok!

↓

valószínüségeket összeadom = 1

~~$|a\rangle = c_1 \cdot |1\rangle +$~~

$|a\rangle = \underset{3}{c_1} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \underset{5}{c_2} \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

szám

$\begin{bmatrix} |a\rangle \end{bmatrix}$

szám

$\begin{bmatrix} \hat{x} \end{bmatrix} \begin{bmatrix} \langle 1| \\ |b\rangle \end{bmatrix}$ szám

$\begin{pmatrix} 3 \\ 5 \end{pmatrix}$

The probability that $|a\rangle$ goes into state $|n\rangle$

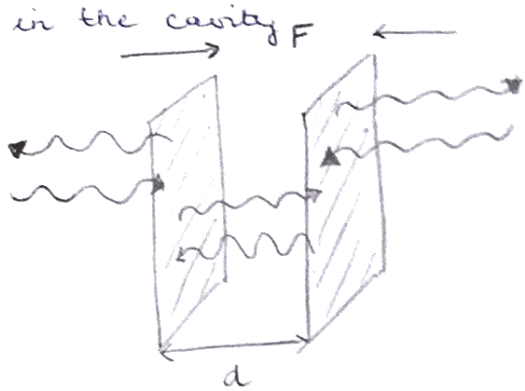
$|c_n|^2 = |\langle n|a\rangle|^2$

Expectation value of measurement

$\langle \hat{A} \rangle = \langle a|\hat{A}|a\rangle$

## 16. Vacuum fluctuations in a cavity - Casimir effect

Two parallel metal plated "mirrors"
↳ there is electromagnetic fluctuation in the cavity
⇓
VACUUM FLUCTUATION




$$F = \frac{\pi \hbar c}{480} \cdot \frac{A}{d^4}$$

$A = 1\,cm^2$, $d = 1\,\mu m$ } $F = 10^{-7}\,N$

$p = \frac{F}{A} = 10^{-3}\,Pa$

$A = 1\,cm^2$, $d = 10\,nm$ } $p = 10^5\,Pa = 1\,atm$

Strongest force between neutral bodies in nature.

### Energy of an EMAG cavity

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

The energy of photon with frequency $\omega$ is $\hbar\omega$.

$\boxed{E_0 = \frac{1}{2}\hbar\omega}$ $\quad E_1 = E_0 + \hbar\omega$ $\quad E_n = E_0 + n\hbar\omega$

+ 1 photon $\quad$ + n photons

↓

without photon in the cavity there is always a half-photon energy.

Spontaneous emission is not property of an isolated atom but it is the property of an atom - vacuum system.

Vacuum is not empty. Zero-point fluctuations are always there.

$$\langle E \rangle = \langle H \rangle = 0$$

$$\Delta E \cdot \Delta H = \langle |E - \langle E \rangle|^2 \rangle \cdot \langle |H - \langle H \rangle|^2 \rangle \geq \frac{\hbar}{2}$$

$$\text{Energy density} = \frac{1}{2}\varepsilon_0 E^2 + \frac{1}{2}\mu_0 H^2 \neq 0$$

Free space vacuum : The atom radiates and decays irreversibly into a lower energy state

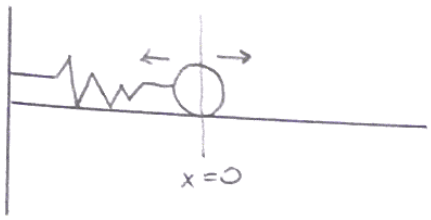
Atom in cavity : Atom exchanges energy with the cavity periodically → jumps down and up between two states.

# 20. Classical and quantum harmonic oscillator



## Classical harmonic oscillator

(motion between two edge values with sinusoidal periodicity)




$F = -C \cdot x$

rugóállandó

$$F = m\ddot{x} = -C \cdot x$$

$$\ddot{x} = -\omega^2 x \qquad \omega = \sqrt{\frac{C}{m}}$$

$x(t) = A \cdot \sin(\omega t) + B \cdot \cos(\omega t)$ kitérés időfüggvény

$\dot{x}(t) = A\omega \cdot \cos(\omega t) - B\omega \cdot \sin(\omega t)$ sebesség időfüggv.

$\ddot{x}(t) = -A\omega^2 \cdot \sin(\omega t) + B\omega^2 \cos(\omega t)$ gyorsulás időfüggv.

$\ddot{x}(t) = -\omega^2 x$

$t = 0, \; x(0) = x_0 \longrightarrow B = x_0$

$t = 0, \; \dot{x}(0) = 0 \longrightarrow A = 0$

$x(t) = x_0 \cdot \cos(\omega t)$

$p(t) = m \cdot \dot{x}(t) = -m \cdot x_0 \cdot \sin(\omega t)$

potenciális energia a hely fgvében

↓

PARABOLA

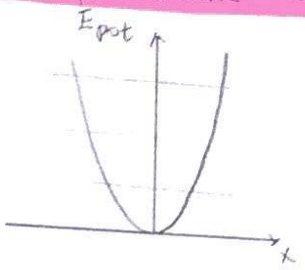
$$E_{pot} = \frac{1}{2} C x^2$$

Heisenberg uncertainty relation:

$\Delta x \cdot \Delta p = 0$ → position and momentum can be accurately measured at the same time

## The quantum harmonic oscillator (PHOTONS)

6/10.




$$\omega = \sqrt{\frac{C}{m}} \qquad u = \sqrt{\frac{\sqrt{Cm}}{\hbar}} \cdot x = \alpha(x) \qquad A_n = \sqrt{\frac{\alpha}{\sqrt{\pi} \cdot 2^n \cdot n!}}$$

Energy eigenvalues

$$E_0 = \frac{1}{2}\hbar\omega \qquad E_1 = \frac{3}{2}\hbar\omega \qquad E_2 = \frac{5}{2}\hbar\omega \quad \dots \quad E_n = \left(\frac{2n+1}{2}\right)\hbar\omega$$

Eigenfunctions

$$\psi_0(u) = A_0 \cdot e^{-\frac{u^2}{2}} \qquad \psi_1(u) = 2 A_1 \cdot u \cdot e^{-\frac{u^2}{2}}$$

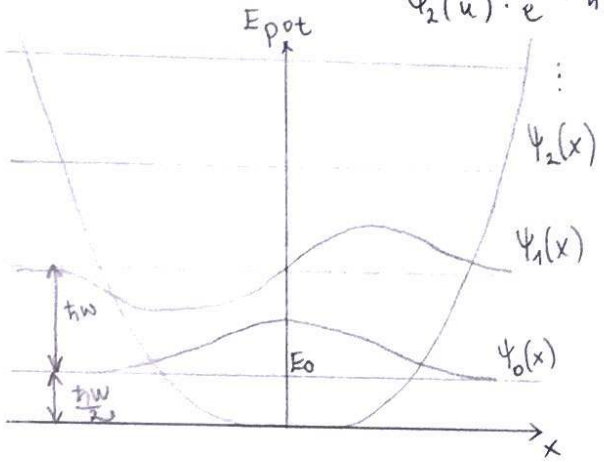
$$\psi_2(u) = 2A_1 \cdot u^2 - 1 \cdot e^{-\frac{u^2}{2}} \quad \dots$$

Stationary eigenstates $\longrightarrow$ no radiation
no oscillation

$$\psi_0(u) \cdot e^{-j\frac{E_0}{\hbar}t}$$

$$\psi_1(u) \cdot e^{-j\frac{E_1}{\hbar}t}$$

$$\psi_2(u) \cdot e^{-j\frac{E_2}{\hbar}t} \quad \dots$$




## Representation by kets.

Eigenvalues: $E_0 = \frac{1}{2}\hbar\omega \qquad E_1 = \frac{3}{2}\hbar\omega \qquad E_2 = \frac{5}{2}\hbar\omega$

Eigenfunctions: $|0\rangle = A_0 \cdot e^{-\frac{u^2}{2}} \qquad |1\rangle = 2A_1 u \cdot e^{-\frac{u^2}{2}} \qquad |2\rangle = 2A_1 u^2 - 1 \cdot e^{-\frac{u^2}{2}}$

$$|n\rangle = A_n \varphi_n(u) \cdot e^{-\frac{u^2}{2}}$$

Hermite polynomials recurrence relation

$$\varphi_0(u) = 1 \qquad \varphi_1(u) = 2u \qquad \varphi_2(u) = 2(u^2 - 1) \dots$$

$$\varphi_n(u) = 2u\varphi_{n-1}(u) - 2(n-1)\varphi_{n-2}(u)$$

Stationary eigenstates:

$$|0\rangle \cdot e^{-j\frac{E_0}{\hbar}t}$$

$$|1\rangle \cdot e^{-j\frac{E_1}{\hbar}t}$$

$$|2\rangle \cdot e^{-j\frac{E_2}{\hbar}t} \quad \dots$$

# I. Time-dependent sinusoidal perturbation of the Hamilton operator of an isolated two-state quantum system.

6/15

## Probability oscillation between states: Rabi oscillation

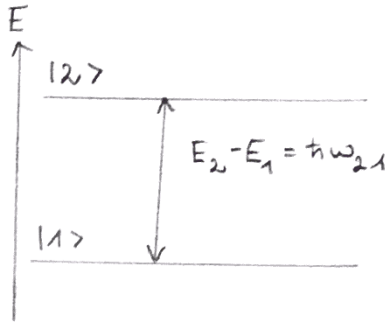
Two-state problem with a sinusoidal oscillating potential can be solved (Semi-classical approximation)

$$\hat{H} = \hat{H}_A + \hat{H}_{Int} \cong \hat{H}_A - \hat{D}\cdot E$$

$\hat{H}_A$: unperturbed Hamilton op. of the two-level atom

$\hat{D}$: atom's dipole moment op.

$E$: electric field at the position of the dipole




unperturbed two-level system:

$$\hat{H}_A = E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2| = \begin{bmatrix} E_1 & 0 \\ 0 & E_2 \end{bmatrix}$$

$$\hat{H}_A|1\rangle = E_1|1\rangle = \hbar\omega_1|1\rangle$$

$$\hat{H}_A|2\rangle = E_2|2\rangle = \hbar\omega_2|2\rangle$$

$$\omega_{21} = \frac{(E_2 - E_1)}{\hbar} = -\omega_{12}$$

Completeness: $|1\rangle\langle 1| + |2\rangle\langle 2| = \hat{1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

Dipole-field interaction: $\hat{H}_{Int} \cong -\hat{D}\cdot E$

$$\hat{D} = \begin{bmatrix} 0 & D \\ D^* & 0 \end{bmatrix}$$ Hermitian operator

dipole moment: $\hat{D} = e\cdot r$

EMAG perturbation: $E(r_0, t) = E\cdot\cos(\omega t)\cdot i$

$$\hat{H}_{Int} = -\underbrace{E(t)}_{\text{electric field in time}}(\gamma_{12}|1\rangle\langle 2| + \gamma_{21}|2\rangle\langle 1|) = -\begin{bmatrix} 0 & E(t)\gamma_{12} \\ E(t)\gamma_{21} & 0 \end{bmatrix}$$

$$\gamma_{12} = e\langle 1|r|2\rangle = |\gamma_{12}|\cdot e^{i\varphi}$$

$$\gamma_{12} = \gamma_{21}^*$$

Rabi frequency: $\Omega_R = \dfrac{|\gamma_{12}|\cdot E}{\hbar}$

Transition between two states: $|1\rangle \rightleftarrows |2\rangle$

Initial state at $t=0$:

$$\left.\begin{aligned} c_1(0) &= 1 \\ c_2(0) &= 0 \end{aligned}\right\} \quad |\psi(0)\rangle = |1\rangle$$

Time-dependent Schrödinger equation:

$$j\hbar \frac{d}{dt} |\Psi(r_0,t)\rangle = \left(\hat{H}_A - e \cdot r \cdot E(r_0,t)\right) \cdot |\Psi(r_0,t)\rangle$$

Solution: $|\Psi(t)\rangle = c_1(t) \cdot |1\rangle + c_2(t) \cdot |2\rangle$

$$|c_1(t)|^2 + |c_2(t)|^2 = 1$$

$$\Psi = \begin{pmatrix} \langle 1|\Psi\rangle \\ \langle 2|\Psi\rangle \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \rightarrow \text{PROBABILITY AMPLITUDES}$$

$|\langle i|\Psi\rangle|^2 = |c_i|^2$ ⇐ the probability of finding the system in state $|i\rangle$

## RWA Rotating Wave Approximation

- two frequencies are present: $\omega_{21} = -\omega_{12} = \frac{(E_2 - E_1)}{\hbar}$ resonance freq. ies transition between two states

  $\omega$: photon frequency $(\omega = \omega_0 + \Delta)$

- dynamics: sum of signals with frequencies:

$\omega_{21} + \omega \rightarrow e^{\pm j(\omega_{21}+\omega)t}$ FAST ← RWA neglects fast terms.

$\boxed{\omega_{21} - \omega \rightarrow e^{\pm j(\omega_{21}-\omega)t} \quad \text{SLOW}}$

## Schrödinger equation in RWA

$$\frac{d}{dt} c_1(t) = -j \frac{\Omega_R}{2} \cdot e^{-j\varphi} \cdot \underbrace{e^{j(\omega-\omega_{21})t}}_{\approx 1} \cdot c_2(t)$$

$$\frac{d}{dt} c_2(t) = -j \frac{\Omega_R}{2} \cdot e^{j\varphi} \cdot \underbrace{e^{-j(\omega-\omega_{21})t}}_{\approx 1} \cdot c_1(t)$$

resonance condition: $\omega = \omega_{21}$

$$\boxed{\frac{d}{dt} c_1(t)} = -j \frac{\Omega_R}{2} \cdot e^{-j\varphi} \cdot c_2(t)$$

$$\frac{d}{dt} c_2(t) = -j \frac{\Omega_R}{2} \cdot e^{j\varphi} \cdot c_1(t)$$

$$\frac{d^2}{dt^2} c_2(t) = -j \frac{\Omega_R}{2} \cdot e^{j\varphi} \cdot \boxed{\frac{d}{dt} c_1(t)} = \underbrace{\overbrace{(-j)}^{-1} \frac{\Omega_R}{2} \cdot e^{j\varphi} \cdot (-j) \frac{\Omega_R}{2} \cdot e^{-j\varphi}}_{\frac{\Omega_R^2}{4}} \cdot c_2(t)$$

$|1\rangle \cdot e^{-j\frac{E_1}{\hbar}t}$

$e^{-j\frac{E_2}{\hbar}t}$

2 2

$$\frac{d^2}{dt^2} c_2(t) = -\frac{\Omega_R^2}{4} \cdot c_2(t)$$

$$c_2(t) = A \cdot e^{j\frac{\Omega_R}{2}t} + B \cdot e^{-j\frac{\Omega_R}{2}t}$$

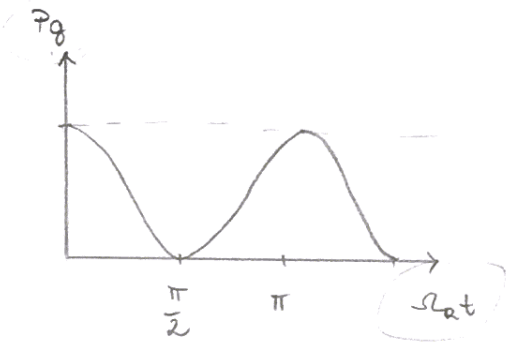
Condition : $c_1(0) = 1$

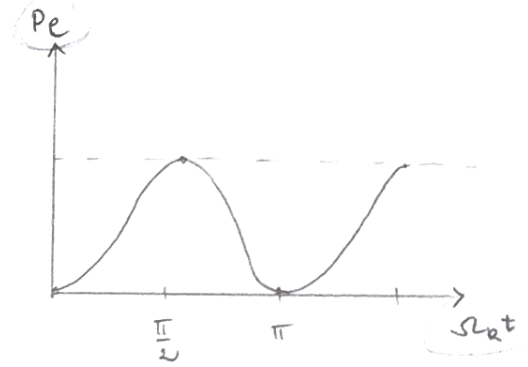
$c_2(0) = 0$

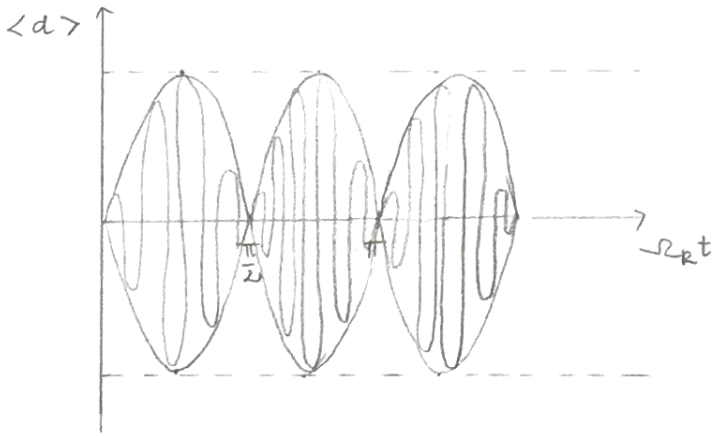
$|c_1(t)|^2 + |c_2(t)|^2 = 1$

$c_1(t) = \cos \frac{\Omega_R}{2} t$ $\qquad P_1(t) = |c_1(t)|^2 = \cos^2(\Omega t)$

$c_2(t) = \sin \frac{\Omega_R}{2} t$ $\qquad P_2(t) = |c_2(t)|^2 = \sin^2(\Omega t)$




Rabi oscillation in two-state quantum system

Time evolution of the system starting in state $|1\rangle$ under the application of an applied monochromatic field shows that the state amplitudes evolve such that :

$$|c_1(t)|^2 = \frac{\Omega^2}{\Omega_R^2} \cdot \sin^2\left(\frac{\Omega_R t}{2}\right)$$

Probability oscillation in time, depending on Rabi-frequency.

$$|c_2(t)|^2 = \frac{\Delta^2}{\Omega_R^2} + \frac{\Omega^2}{\Omega_R^2} \cdot \cos\left(\frac{\Omega_R t}{2}\right)$$

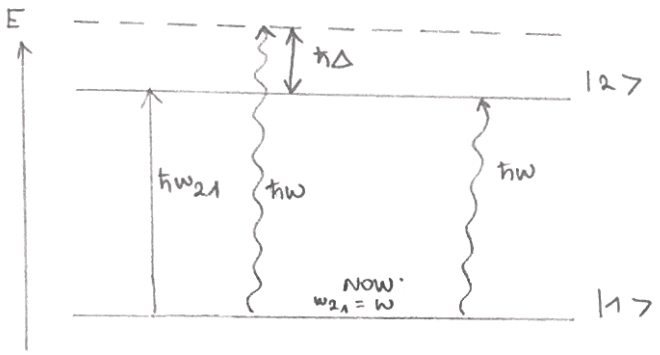
$$\Omega_R^2 = \Omega^2 + \underbrace{\Delta^2}_{\text{now it is zero}}$$

Probabilities to be in state $|1\rangle$ or $|2\rangle$ oscillate with frequency $\Omega_R$.

$\Omega = \frac{\mu E_0}{\hbar}$ ↓ coupling strength

$\Delta = \omega - \omega_0$ ↓ detuning

$\Rightarrow$ $\Omega$ and $\Delta$ parameters define the system at the end.




The applied field can induce transitions between two states for frequency not exactly on resonance freq.

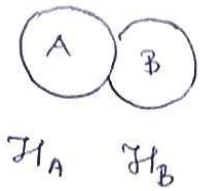
$\Delta \neq 0$

↓

probability amplitude is shorter.

4

## Composite closed quantum system




**Hilbert space of composite system:**

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$$

tensor product

$$\left.\begin{array}{l}\dim N_A \\ \dim N_B\end{array}\right\} \mathcal{H}_A \otimes \mathcal{H}_B \quad \dim N = N_A + N_B$$

$$\left.\begin{array}{l}|a\rangle \in \mathcal{H}_A \\ |b\rangle \in \mathcal{H}_B\end{array}\right\} \underset{\in \mathcal{H}_A \otimes \mathcal{H}_B}{|a\rangle \otimes |b\rangle} \Leftrightarrow |a,b\rangle$$

Whether a system is composite or not it depends on the definition.

All systems become composite when we try to describe the effects of the environment, leading to relaxation and decoherence.

**Microscopic system:**

Hilbert space is a "democratic world" with equal opportunities to all states. All superpositions of states represent possible state of the system.

**Macroscopic environment:**

There are states called POINTER STATES, which survive environment effect. Most of the states are more fragile and their coherence vanish in a short time.

**Two-body composite system problem**

Two particles eigenstates: $|1_1\rangle, |2_1\rangle \dots$

$|1_2\rangle, |2_2\rangle \dots$

**After interaction:**

composite eigenstates are superposition of tensor products of component eigenstates:

$$|1,2\rangle = c_1 |1_1\rangle \otimes |1_2\rangle + c_2 |2_1\rangle \otimes |2_2\rangle$$

**Hamilton operator:** $\hat{H} = \hat{H}_1 \otimes \hat{1}_{N_2} + \hat{H}_2 \otimes \hat{1}_{N_1} + \hat{H}_{int}$.

If $\hat{H}_{int} = 0$, then the solution of Schrödinger equation: $|\psi(t)\rangle = |\psi_1(t)\rangle \otimes |\psi_2(t)\rangle$

14. Isolated, closed and composite quantum systems.

Isolated quantum system described by a Hamiltonian $\hat{H}_0$ independent of time

$$j\hbar \frac{\partial}{\partial t} |\psi\rangle = H_0 |\psi\rangle$$

$$H_0 |n\rangle = E |n\rangle$$

time-dependence: $e^{j\frac{E}{\hbar}t}$

superposition: $|\psi(t)\rangle = \sum_n c_n(t) |n\rangle$

Energy spectrum: $E_1, E_2, \dots, E_n$

$Z_1, Z_2, \dots, Z_n$

Orbitals: $|1\rangle, |2\rangle, \dots, |n\rangle, \dots, |m\rangle$

$\langle n|m\rangle = \delta_{ij}$

(orthonormality)

If the system is initially prepared in eigenstate $|n\rangle$ of $H_0$, then the probability of finding it later in state $|m\rangle$ of $H_0$, if $m \neq n$:

$$P_{n\to m}(t) = |\langle m|\psi(t)\rangle|^2 = \emptyset$$

→ initial $|n\rangle$ eigenstate → $|m\rangle$ eigenstate

$P_{|n\rangle \to |m\rangle}(t) = \emptyset$ because of orthogonality

→ initial $|n\rangle$ eigenstate → $|\psi\rangle$ state

$P_{|n\rangle \to |\psi\rangle}(t) = \emptyset$ because it will remain in eigenstate that is stable, if the atom is not coupled to the environment. (collision / coupling emag)

Closed system is time-dependent:

$$j\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{H}(t) |\psi\rangle$$

15. A two-state atom in a cavity.
The Jaynes - Cummings Model.

Approximate model of an open quantum optics system

System composed of a two-level (two-state) atom interacting with a quantized mode of an optical cavity.

Emag radiation can leak from the cavity (photon loss).

The walls of the cavity can absorb energy (dissipation).

$$|e\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad |g\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

PROJECTION OPERATOR

$$\hat{\sigma}_+ = |e\rangle\langle g| = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \qquad \hat{\sigma}_- = |g\rangle\langle e| = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

$$\hat{\sigma}_+ |g\rangle = |e\rangle\langle g|g\rangle = |e\rangle \qquad \hat{\sigma}_- |e\rangle = |g\rangle\langle e|e\rangle = |g\rangle$$

$$\hat{H}_{atom} = E_1 |e\rangle\langle e| + E_2 |g\rangle\langle g| = \begin{bmatrix} E_1 & 0 \\ 0 & E_2 \end{bmatrix} =$$

$$= \frac{1}{2}\begin{bmatrix} E_1 + E_2 & 0 \\ 0 & E_1 + E_2 \end{bmatrix} + \frac{1}{2}\begin{bmatrix} (E_1 - E_2) & 0 \\ 0 & -(E_1 - E_2) \end{bmatrix} = \frac{1}{2} \cdot \Delta E \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\hat{H}_{atom} = \frac{1}{2} \hbar \omega_a \hat{\sigma}_z \qquad \hat{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\hat{H} = \hat{H}_{atom} + \hat{H}_{radiation} + \hat{H}_{interaction}$$

$$\hat{H}_{atom} = \sum_i E_i |i\rangle\langle i| = \frac{1}{2} \hbar \omega_a \hat{\sigma}_z$$

$$\hat{H}_{rad} = \sum_l \hbar \omega_{cl} \left( \frac{1}{2} + \hat{a}_l^\dagger \hat{a}_l \right) \cong \hbar \omega_c \, \hat{a}^\dagger \hat{a}$$

CREATION OPERATOR

ANNIHILATION OPERATOR

$$\hat{H}_{int} = \hbar \lambda \left( \hat{\sigma}_+ \hat{a} + \hat{\sigma}_- \hat{a}^\dagger \right)$$

# 11. Pure and mixed states of a quantum system. Density matrix.

## Pure and mixed states of field and matter

**Example 1:** single photon in a polarization

$$|\psi\rangle = c_H|H\rangle + c_V|V\rangle$$

H: horizontally polarized photon state

V: vertically pol. photon state

$$|c_H|^2 + |c_V|^2 = 1$$

$\Rightarrow$ PURE STATE

Any field or matter for which we know that $|\psi\rangle = \sum_n c_n|n\rangle$ is said to be a quantum object in a pure state.

**Example 2:** beam of light that is a mixture from two different and quite independent lasers: laser 1 and laser 2

The probability that a given photon is from laser 1 is $P_1$ or from laser 2 is $P_2$.

The two lasers give photons of two different polarization state $\psi_1$ and $\psi_2$.

A polarizing filter in any specific state, it will not pass 100% of either set of photons.

Linear combination cannot be written because that would violate our presumption that the lasers are independent.

We can only describe pure state of the two lasers if the photons were actually both in the same mode (frequency and spatial form)

$\Rightarrow$ MIXED STATE

Probabilities: $P_j$

Pure states: $|\psi_j\rangle$

**Density operator of mixed state:**

$$\rho = \sum_j P_j |\psi_j\rangle\langle\psi_j|$$

$\rightarrow$ $\rho$ is representing the state, not a physical observable in this case.

The ensemble average expectation value for an observable in mixed state :

6/16

$$\langle \bar{\hat{A}} \rangle = \sum_j P_j \langle \psi_j | \hat{A} | \psi_j \rangle$$

Properties of the density matrix $\rho$ :

1.) Density matrix is Hermitian :

$$\rho_{nm} = \sum_j P_j \cdot c_n^{(j)} (c_m^{(j)})^* = \rho_{mn}^* = \sum_j P_j \cdot c_m^{(j)} (c_n^{(j)})^* \quad \text{(complex conjugate)}$$

2.) Diagonal elements give the probabilities of finding the system in a basis state $|m\rangle$ in the mixed state is :

$$\rho_{mm} = \sum_j P_j \, c_m^{(j)} \cdot (c_m^{(j)})^* = \sum_j P_j \, |c_m^{(j)}|^2$$

← real numbers in the diagonal position

3.) Sum of diagonal elements is 1 :
(TRACE)

$$Tr(\rho) = \sum_m \rho_{mm} = \sum_m \sum_j P_j \, |c_m^{(j)}|^2 = \sum_j P_j \cdot \sum_m |c_m^{(j)}|^2 = \sum_j P_j = 1$$

We consider an operator corresponding to a physical observable $\hat{A}$, the product with the density matrix is $\rho\hat{A}$ :

$$\rho\hat{A} = \sum_{m,n} \sum_j P_j \, c_m^{(j)} (c_n^{(j)})^* \, |m\rangle\langle n| \hat{A}$$

Diagonal element of $\rho\hat{A}$ :

$$\langle k | \rho\hat{A} | k \rangle = \sum_{m,n} \sum_j P_j \cdot c_m^{(j)} \cdot (c_n^{(j)})^* \langle k|m\rangle \langle n|\hat{A}|k\rangle =$$

$$= \sum_{m,n} \sum_j P_j \, c_m^{(j)} \cdot (c_n^{(j)})^* \cdot \delta_{km} \langle n|\hat{A}|k\rangle$$

$$Tr(\rho\hat{A}) = \sum_k \langle k|\rho\hat{A}|k\rangle = \sum_j P_j \Big( \sum_m (c_m^{(j)})^* \langle m| \Big) \hat{A} \Big( \sum_k c_k^{(j)} |k\rangle \Big) = \sum_j P_j \langle \psi_j | \hat{A} | \psi_j \rangle$$

$$\Rightarrow \langle \bar{\hat{A}} \rangle = \sum_j P_j \langle \psi_j | \hat{A} | \psi_j \rangle = Tr(\rho\hat{A})$$

The sum of diagonal elements of $\rho\hat{A}$ matrix is the ensemble average expectation value for observable $\hat{A}$.

The trace is independent of the basis → the basis could be any set that is complete for the problem, a complete orthonormal basis.

If the system is in pure state $\psi$, in which $P = 1$ and there is no probability for any other state :

$$Tr(\rho \hat{A}) = \langle \psi | \hat{A} | \psi \rangle = \langle \hat{A} \rangle$$

13. Time - evolution of the density matrix SEE ALSO TOPIC 11.

6/17

The von Neumann - Liouville equation

Density matrix of a mixed state:

$$\rho = \sum_j P_j \underbrace{|\psi_j\rangle\langle\psi_j|}_{\text{matrix, pure state operator}}$$

$P_j$ → classical probabilities → it expresses our ignorance of the environment

Time evolution of a pure state $|\psi_j\rangle$

$$\hat{H}|\psi_j\rangle = j\hbar \frac{\partial}{\partial t}|\psi_j\rangle$$

SCHRÖDINGER EQUATION

Time evolution of a mixed state $\rho(t)$

$$\frac{\partial \rho}{\partial t} = \frac{j}{\hbar}[\rho, \hat{H}]$$

VON NEUMANN - LIOUVILLE EQUATION

10. Multiple electrons in an isolated quantum system.

Exchange energy.

Slater determinant.

Pauli principle.

Isolated quantum system $\rightarrow$ $\hat{H}_0$: time-independent Hamiltonian

$$j\hbar \frac{\partial}{\partial t} |\Psi\rangle = \hat{H}_0 |\Psi\rangle$$

$$\Downarrow$$

$$\hat{H}_0 |n\rangle = E |n\rangle$$

time-dependence: $e^{j\frac{E_n}{\hbar}t}$

$\rightarrow$ any state can be described by the linear combination of eigenstates.

$$|\Psi(t)\rangle = \sum_n c_n(t) \cdot |n\rangle$$

Energy spectrum: $E_1, E_2, \dots, E_i, \dots$

EIGENVALUES $\quad Z_1, Z_2, \dots, Z_i, \dots$

Orbitals: $|1\rangle, |2\rangle, \dots, |n\rangle, \dots, |m\rangle$

EIGENVECTOR

$$\langle n|m\rangle = \delta_{ij} \begin{cases} 1 & i=j \\ 0 & i \neq j \end{cases}$$ orthonormal eigenvectors

If system is initially prepared in eigenstate $|n\rangle$ of $\hat{H}_0$, then the probability of finding it later in state $|m\rangle$ is zero, if there is no exterior environment

$$P_{n\rightarrow m}(t) = |\langle m|\Psi(t)\rangle|^2 = 0$$

Multiple identical particles $\rightarrow$ n-electron problem

In quantum mechanics particles can be absolutely identical (in contrast to classical mechanics). There is no difference if we swap the electrons.

Wavefunction $\Psi$ itself cannot be measured, but there are contexts we can assume.

$$(H_1 + H_2) \cdot \Psi(r_1, r_2) + E_{pot}(r_1, r_2) \cdot \Psi(r_1, r_2) = E \cdot \Psi(r_1, r_2) \qquad (*)?$$

$$\Psi(r_2, r_1) = a \cdot \Psi(r_1, r_2) = a^2 \cdot \Psi(r_2, r_1)$$

$$a^2 = 1$$

$$a = +1 \qquad a = (-1)$$

$$\Psi(r_2, r_1) = \Psi(r_1, r_2) \qquad \Psi(r_2, r_1) = -\Psi(r_1, r_2)$$

$\Rightarrow$ In the case of two identical particles the eigenvalue-problem can be solved, if we swap them $\rightarrow$ the eigenvalues will not change, the difference between the eigenfunctions will be $a^2$ variable.

## BOSONS

- symmetric $\psi$

  $a = +1$

  $\psi(r_2, r_1) = \psi(r_1, r_2)$

- integer spin : $\pm 1$
- e.g. photon

## FERMIONS

- asymmetric $\psi$

  $a = (-1)$

  $\psi(r_2, r_1) = -\psi(r_1, r_2)$

- half-integer spin : $\pm 1/2$
- eg. electron

Single electron wavefunctions: $\psi_a(r), \psi_b(r)$

identical, undistinguishable particles

- $\psi(1,2) = \frac{1}{\sqrt{2}} \cdot (\psi_a(1)\psi_b(2) + \psi_a(2)\psi_b(1)) =$

  $= \psi(2,1)$

- $\psi(1,2) = \frac{1}{\sqrt{2}} \cdot (\psi_a(1)\psi_b(2) - \psi_a(2)\psi_b(1)) =$

  $= \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_a(1) & \psi_a(2) \\ \psi_b(1) & \psi_b(2) \end{vmatrix} = -\psi(2,1)$

  normalization constant

**SLATER DETERMINANT**

$\Downarrow$

**PAULI PRINCIPLE**

1-essel jelölt $e^-$, a bekapcsolt van

"N" elektron különböző bekapcsolt

(N)

$$\psi(1,2,\dots,N) = \frac{1}{\sqrt{N!}} \cdot \begin{vmatrix} \psi_1(1) & \psi_1(2) & \dots & \psi_1(N) \to \psi_1(r) \\ \psi_2(1) & \psi_2(2) & \dots & \psi_2(N) \to \psi_2(r) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_N(1) & \psi_N(2) & \dots & \psi_N(N) \to \psi_N(r) \end{vmatrix}$$

it describes the wavefunction of a multi-fermionic system.

<u>Pauli principle</u>: two identical fermions cannot be in the same quantum state at the same time.

**The solution of the N-electron problem is reduced to N single $e^-$ problem**

Solution of time-independent Schrödinger equation:

$$\hat{H}_0 \psi(r) = E \cdot \psi(r) \qquad H = \sum_i H_i = \sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m_i}\Delta_i + E_{ipot}(r_i)\right)$$

$$\psi(r_1, r_2, \dots, r_N) = \psi_1(r_1) \cdot \psi_2(r_2) \cdot \dots \cdot \psi_N(r_N)$$

$$\psi_2 \dots \psi_N \cdot \underbrace{H_1\psi_1} + \psi_1 \dots \psi_3 \cdot \underbrace{H_2\psi_2} + \dots + \psi_1\psi_2 \dots \psi_{N-1} \cdot \underbrace{H_N\psi_N} = E \cdot \psi_1\psi_2 \dots \psi_N \quad / : (\psi_1 \cdot \psi_2 \cdot \dots \psi_N)$$

$$\frac{1}{\psi_1(r_1)} \cdot H_1 \cdot \psi_1(r_1) + \frac{1}{\psi_2(r_2)} \cdot H_2 \cdot \psi(r_2) + \dots + \frac{1}{\psi_N(r_N)} \cdot H_N \cdot \psi_N(r_N) = E$$

$$H_1 \cdot \psi_1(r_1) = E_1 \cdot \psi_1(r_1)$$

$$H_2 \cdot \psi_2(r_2) = E_2 \, \psi_2(r_2)$$

$$\vdots$$

$$H_N \cdot \psi_N(r_N) = E_N \cdot \psi_N(r_N)$$

The energy of the N-electron system:

$$E = E_1 + E_2 + \ldots + E_N$$

Solutions:

$$\psi(r_1, r_2, \ldots, r_N) = \sum_i c_i \cdot \psi_{1i}(r_1) \cdot \psi_{2i}(r_2) \cdot \ldots \cdot \psi_{Ni}(r_N)$$

$$\underbrace{c_1 \cdot \psi_{11}(r_1)\psi_{21}(r_2)\ldots\psi_{N1}(r_N)}_{\text{Slater-det rows multiplicated}} + c_2 \; \psi_{12}(r_1) \cdot \psi_{22}(r_2) \ldots \psi_{N2}(r_N)$$

"cserélő energia"

Exchange energy:

Suppose we have two electrons in identical spin states.

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\nabla_{r_1}^2 + \nabla_{r_2}^2\right) + \frac{e^2}{4\pi\varepsilon_0 |r_1 - r_2|} \qquad \hat{H} = -\frac{\hbar^2}{2m}\Delta + E_{pot}$$

kétszer hullámfüggvény a elektronnak

$$\psi(r_1, r_2) = \frac{1}{\sqrt{2}}\left[\psi_a(r_1)\psi_b(r_2) - \psi_a(r_2)\psi_b(r_1)\right]$$

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|1,a\rangle|2,b\rangle - |2,a\rangle|1,b\rangle\right)$$

$$\langle E\rangle = \langle\psi|\hat{H}|\psi\rangle = \frac{1}{2}\cdot\left[\begin{array}{l}\langle 1,a|\langle 2,b|\hat{H}|1,a\rangle|2,b\rangle + \langle 2,a|\langle 1,b|\hat{H}|2,a\rangle|1,b\rangle - \\ -\langle 1,a|\langle 2,b|\hat{H}|2,a\rangle|1,b\rangle - \langle 2,a|\langle 1,b|\hat{H}|1,a\rangle|2,b\rangle\end{array}\right]$$

$$\langle 1,a|\cdot\langle 2,b|\hat{H}|1,a\rangle\cdot|2,b\rangle = -\frac{\hbar^2}{2m}\cdot\langle 1,a|\langle 2,b|\nabla_{r_1}^2|1,a\rangle\cdot|2,b\rangle -$$

$$-\frac{\hbar^2}{2m}\langle 1,a|\langle 2,b|\nabla_{r_2}^2|1,a\rangle\cdot|2,b\rangle +$$

$$+\langle 1,a|\langle 2,b|\cdot\frac{e^2}{4\pi\varepsilon_0|r_1 - r_2|}\cdot|1,a\rangle|2,b\rangle$$

1.

$$-\frac{\hbar^2}{2m}\langle 1,a|\langle 2,b|\nabla_{r_1}^2|1,a\rangle|2,b\rangle = -\frac{\hbar^2}{2m}\langle 1,a|\nabla_{r_1}^2|1,a\rangle\underbrace{\langle 2,b|2,b\rangle}_{=1}$$

$$-\frac{\hbar^2}{2m}\langle 1,a|\nabla^2_{r_1}|1,a\rangle = -\frac{\hbar^2}{2m}\int \psi_a^*(r)\,\nabla^2\psi_a(r)\,dr^3 = E_{kinEa}$$

2.

$$-\frac{\hbar^2}{2m}\langle 2,b|\nabla^2_{r_2}|2,b\rangle = -\frac{\hbar^2}{2m}\int \psi_b^*(r)\,\nabla^2\psi_b(r)\,dr^3 = E_{kinEb}$$

$$\langle 1,a|1,a\rangle = 1$$

3.

$$E_{potEab} = e^2\int \frac{|\psi_a(r)|^2\cdot|\psi_b(r')|^2}{4\pi\varepsilon_0|r-r'|}\,dr^3\,dr'^3$$

$$\langle E\rangle = \langle\psi|\hat{H}|\psi\rangle = \frac{1}{2}\left[\begin{array}{l} E_{kinEa} + E_{kinEb} + E_{potEab} + \\ -\langle 1,a|\langle 2,b|\hat{H}|2,a\rangle|1,b\rangle - \langle 2,a|\langle 1,b|\hat{H}|1,a\rangle|2,b\rangle \end{array}\right]$$

$$\Rightarrow \quad \langle 2,a|\langle 1,b|\hat{H}|1,a\rangle|2,b\rangle = [\langle 1,a|\langle 2,b|\hat{H}|2,a\rangle|1,b\rangle]^*$$

$$E_{exchange-ab} = -Re\left[\int \psi_a^*(r_1)\psi_b^*(r_2)\cdot\hat{H}\cdot\psi_a(r_2)\psi_b(r_1)\,dr_1^3\,dr_2^3\right]$$

$$\langle E\rangle = E_{kinEa} + E_{kinEb} + E_{potEab} + \boxed{E_{exchange-ab}}$$

$$|\psi_{different}\rangle = |1,a\rangle|2,b\rangle\ldots|N,n\rangle$$

PARTICLES SINGLE PARTICLE STATES

* identical particles = indistinguishable

6. Quantum - classical models of matter - field interaction.
Time - independent perturbation of the stationary states of isolated quantum systems.
First order approximation.

(I.) Interaction dynamics:
Quantum - classical model
→ classical fields are perturbating a quantum mechanical system

time - independent
STATIC

$\hat{H}_{Int} = \hat{V}$

time - dependent

$\hat{H}_{Int}(t)$

(II) Quantum - quantum model
Interaction of the quantized field (photons) with quantized matter.

Time - independent perturbation of stationary states

$(\hat{H}_0 + \hat{H}') |\psi_n\rangle = (\hat{H}_0 + \lambda \hat{V}) |\psi_n\rangle = E_n |\psi_n\rangle$ ⇐ perturbated system
(stationary + weak EMAG field)

Expand the unknowns:

$|\psi\rangle = |\psi_0\rangle + \lambda |\psi_1\rangle + \lambda^2 |\psi_2\rangle + \dots$

$E = E_0 + \lambda E_1 + \lambda^2 E_2 + \dots$

$(\hat{H}_0 + \lambda \hat{V})(|\psi_0\rangle + \lambda|\psi_1\rangle + \lambda^2|\psi_2\rangle + \dots) = (E_0 + \lambda E_1 + \lambda^2 E_2 + \dots)(|\psi_0\rangle + \lambda|\psi_1\rangle + \lambda^2|\psi_2\rangle + \dots)$

$\hat{H}_0|\psi_0\rangle + \lambda(\hat{H}_0|\psi_1\rangle + \hat{V}|\psi_0\rangle) + \lambda^2(\hat{H}_0|\psi_2\rangle + \hat{V}|\psi_1\rangle) + \dots =$

$= E_0|\psi_0\rangle + \lambda(E_0|\psi_1\rangle + E_1|\psi_0\rangle) + \lambda^2(E_0|\psi_2\rangle + E_1|\psi_1\rangle + E_2|\psi_0\rangle) + \dots$

$\lambda^0 \rightarrow \hat{H}_0|\psi_0\rangle = E_0|\psi_0\rangle$

$\lambda^1 \rightarrow \hat{H}_0|\psi_1\rangle + \hat{V}|\psi_0\rangle = E_0|\psi_1\rangle + E_1|\psi_0\rangle$

$\lambda^2 \rightarrow \hat{H}_0|\psi_2\rangle + \hat{V}|\psi_1\rangle = E_0|\psi_2\rangle + E_1|\psi_1\rangle + E_2|\psi_0\rangle$

$E_m = E_m^0 + \langle m|\hat{V}|m\rangle = E_m^0 + V_{mm}$

$$|\psi_m\rangle = |m\rangle + \sum_{k \neq m} \frac{\langle k|\hat{V}|m\rangle}{E_m^0 - E_k^0} \cdot |k\rangle$$

unperturbated

$E_1^0$

$E_2^0$

$\vdots$

$|1\rangle$

$|2\rangle$

$\vdots$

perturbated

$$E_1 = E_1^0 + \langle 1|\hat{V}|1\rangle$$

$$E_2 = E_2^0 + \langle 2|\hat{V}|2\rangle$$

$$\vdots$$

$$|\psi_1\rangle = |1\rangle + \sum_{k\neq 1} \frac{\langle k|\hat{V}|1\rangle}{E_1^0 - E_k^0}$$

$$|\psi_2\rangle = |2\rangle + \sum_{k\neq 2} \frac{\langle k|\hat{V}|2\rangle}{E_2^0 - E_k^0} \cdot |k\rangle$$

$\hat{V}$ perturbation operator

$$\begin{bmatrix} \langle 1|\hat{V}|1\rangle & \langle 1|\hat{V}|2\rangle & \langle 1|\hat{V}|3\rangle & \cdots \\ \langle 2|\hat{V}|1\rangle & \langle 2|\hat{V}|2\rangle & \langle 2|\hat{V}|3\rangle & \cdots \\ \langle 3|\hat{V}|1\rangle & \langle 3|\hat{V}|2\rangle & \langle 3|\hat{V}|3\rangle & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

$$\langle n|\hat{V}|m\rangle = \int_{\substack{\text{configuration} \\ \text{space}}} \psi_n^* \cdot \hat{V} \cdot \psi_m \, dq_1 \cdots dq_f$$