Schrödingerjeva enačba

Dejstva:

- $E = \hbar\omega = h\nu$ $\qquad \hbar = \frac{h}{2\pi}$ $\qquad$ Planck, Einstein
- $p = \hbar k$ $\qquad k$ ... valovni vektor $\qquad k = \frac{2\pi}{\lambda}$ $\qquad$ de Broglie
- Prost delec $\qquad E = \frac{p^2}{2m}$
- valovanje

Kakšne enačbe že poznamo?

- valovna enačba

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} \qquad u = u_0 \cos(kx - \omega t) \qquad \Rightarrow \omega = \pm c k$$

$$\Rightarrow E \propto p \qquad ✗$$

Ni v redu

- difuzijska enačba

$$D\frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial t} \qquad T = T_0 \cos kx \cos \omega t$$

nastavek

$$-k^2 D\, T(x,t) = -\omega T_0 \sin(\omega t)\cos(kx) \not\propto T(x,t) \qquad ✗$$

$$T = T_0 e^{i(kx-\omega t)}$$

nastavek

$$k^2 D = i\omega \qquad \omega, k \in \mathbb{R} \quad ; \quad D = ? \in \mathbb{C}$$

Naj bo $\qquad D = \frac{i\omega}{k^2} = \frac{i\, k^2\hbar^2}{\hbar\, 2m k^2} = i\frac{\hbar}{2m}$

$$\hookrightarrow E = \frac{p^2}{2m} \quad ✓$$

$$\Rightarrow \quad \boxed{i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi} \qquad \psi = \psi_0 e^{i(kx-\omega t)}$$

Rešitev za prost delec

Kaj je ψ?

$$\psi = \alpha + i\beta \qquad \alpha, \beta \in \mathbb{R}$$

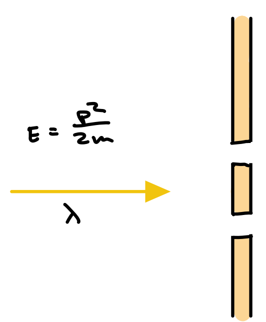
$$i\hbar(\dot\alpha + i\dot\beta) = -\frac{\hbar^2}{2m}(\alpha'' + i\beta'') + V(\alpha + i\beta)$$

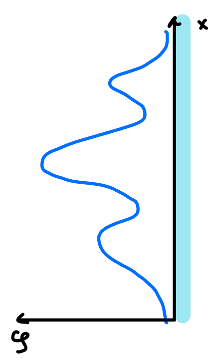
Re: $\quad -\hbar\dot\beta = -\frac{\hbar^2}{2m}\alpha'' + V\alpha$ $\qquad$ Schrödingerjeva enačba

Im: $\quad \hbar\dot\alpha = -\frac{\hbar^2}{2m}\beta'' + V\beta$ $\qquad$ v realnem

Max Born $\qquad |\psi^2(x,t)| = \rho(x,t) = \alpha^2(x,t) + \beta^2(x,t)$ $\qquad$ Verjetnostna amplituda

$$dP(\vec{r}, t) = \rho\, dV$$





Kaj je $\vec{r}$ oz. x?

- ni koordinata delca
- temveč pozicija kjer lahko najdemo delec

Kontinuitetna enačba za verjetnost

Delec je nekje

$$P = \int_{-\infty}^{\infty} \rho(x,t)\, dx = 1 \qquad \forall t$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{j} = q \qquad \text{kontinuitetna enačba (splošna)}$$

$$\frac{\partial}{\partial t} |\psi|^2 = \frac{\partial \psi^*}{\partial t}\psi + \psi^* \frac{\partial \psi}{\partial t} =$$

kompleksno konjugirano

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi$$

$$= -\frac{\hbar^2}{2m(-i\hbar)}\left(\frac{\partial^2 \psi^*}{\partial x^2}\right)\psi + \frac{V^*}{-i\hbar}\psi^*\psi + c.c.$$

$$i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi^*}{\partial x^2} + V^*\psi^*$$

$$\left(\frac{\partial^2}{\partial x^2}\psi^*\right)\psi = \frac{\partial}{\partial x}\left(\frac{\partial \psi^*}{\partial x}\psi\right) - \frac{\partial \psi^*}{\partial x}\frac{\partial \psi}{\partial x}$$

$$\frac{\partial}{\partial t}|\psi|^2 = -\frac{\partial}{\partial x}\Big(\underbrace{\frac{\hbar}{2im}\left(\psi^*\frac{\partial \psi}{\partial x} - \psi\frac{\partial \psi^*}{\partial x}\right)}_{j_x}\Big)\underbrace{-\frac{2}{\hbar}\,\mathrm{Im}\,V\,|\psi|^2}_{q}$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} j_x = q$$

$$\vec{j} = \frac{\hbar}{2mi}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)$$

optični potencial

$$q = -\frac{2}{\hbar}\,\mathrm{Im}\,V\,\rho = 0$$

izvor

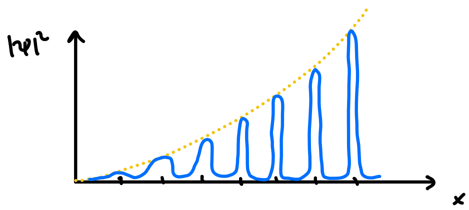
če ni izvorov

Lastnosti valovne funkcije

① $\int_{-\infty}^{\infty} |\psi|^2\, dx = 1 \qquad \psi \in \mathbb{C}$

② ψ je zvezna, $\frac{\partial}{\partial x}\psi$

③ kako je pri $|x| \to \infty$?



$$\psi = c\, x^2 e^{-x^2 \sin^2 x}$$

po navadi $|\psi|^2 \xrightarrow{|x|\to\infty} 0$

Schwartzov prostor: $\int_{-\infty}^{\infty} x^n |\psi|^2\, dx < \infty$

↳ primeri $\quad \psi = f(x)\, e^{-\lambda x}$

$e^{-\lambda x^2}$

④ $$i\hbar \frac{\partial}{\partial t}\int_a^b \psi\, dx = -\frac{\hbar^2}{2m}\int_a^b \frac{\partial^2 \psi}{\partial x^2}\, dx + \int_a^b V\psi\, dx$$

$b \to a$ $$i\hbar \frac{\partial \psi}{\partial t}(b-a) = -\frac{\hbar^2}{2m}\frac{\partial \psi}{\partial x}\Big|_a^b + \psi\int_a^b V\, dx$$

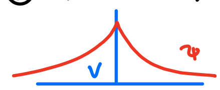
$\downarrow$ 0

$$0 = -\frac{\hbar^2}{2m}\left(\psi'(b) - \psi'(a)\right) + \psi \cdot$$

$V = ?$

ⓐ V zvezen $\to \int_a^b V\,dx = 0 \to \psi'$ zvezen

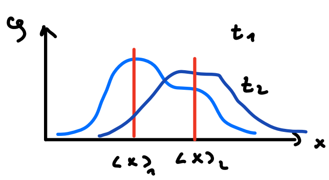
ⓑ $V(x) = \lambda\,\delta(x)$



ψ' ni zvezen

⑤ ψ'' če ima V skok v x ga ima tudi ψ''.

Hitrost težišča porazdelitve



$$\langle x \rangle = \int x\,\rho\, dx = \int x\,\psi^*\psi\, dx = \int \psi^*\, x\, \psi\, dx$$

povprečna vrednost $\bar{x}$

pričakovana vrednost $\langle x \rangle$

hitrost težišča $$v_T = \frac{d}{dt}\langle x\rangle = \int_{-\infty}^{\infty}\left(\frac{\partial \psi^*}{\partial t}\, x\, \psi + \psi^* \underbrace{\frac{\partial x}{\partial t}}_{=0}\psi + \psi^* x \frac{\partial \psi}{\partial t}\right)dx$$

$$\overset{SE}{=} \frac{\hbar^2}{2mi\hbar}\int_{-\infty}^{\infty}\left(\frac{\partial^2\psi^*}{\partial x^2}\, x\, \psi - c.c.\right)dx$$

$$\frac{\partial^2\psi^*}{\partial x^2}\, x\, \psi = \frac{\partial}{\partial x}\left(\frac{\partial\psi^*}{\partial x}\, x\, \psi\right) - \frac{\partial\psi^*}{\partial x}\overset{1}{\frac{\partial x}{\partial x}}\psi - \frac{\partial\psi^*}{\partial x}\, x\, \frac{\partial\psi}{\partial x} =$$

$$= \frac{\partial}{\partial x}\left(\frac{\partial\psi^*}{\partial x}\, x\, \psi\right) - \frac{\partial}{\partial x}(\psi^*\psi) + \psi^*\frac{\partial}{\partial x}\psi - \frac{\partial}{\partial x}\left(\psi^*\, x\, \frac{\partial\psi}{\partial x}\right) + \psi^*\frac{\partial\psi}{\partial x} + \psi^*\, x\, \frac{\partial^2\psi}{\partial x^2}$$

$$v_T = \frac{\hbar^2}{2i\hbar m}\int_{-\infty}^{\infty}\frac{\partial}{\partial x}\underbrace{\left(\frac{\partial\psi^*}{\partial x}\, x\, \psi - |\psi|^2 - \psi^*\, x\, \frac{\partial\psi}{\partial x}\right)dx}_{\to 0} + \frac{1}{m}\int_{-\infty}^{\infty}\psi^*\left(-i\hbar\frac{\partial}{\partial x}\psi\right)dx =$$

$$\boxed{\langle p\rangle = m\frac{d\langle x\rangle}{dt} = \int_{-\infty}^{\infty}\psi^*\,\hat p\,\psi\, dx}$$

$\hat p = -i\hbar\frac{\partial}{\partial x}$ $\qquad$ $\hat{\vec p} = -i\hbar\nabla$

Operator gibalne količine

Operatorji

$\hat p = -i\hbar\frac{\partial}{\partial x}$ $\qquad$ $\hat p^2 = \hat p\hat p = -i\hbar\frac{\partial}{\partial x}\left(-i\hbar\frac{\partial}{\partial x}\right) = -\hbar^2\frac{\partial^2}{\partial x^2}$ $\qquad$ $\hat p^n = (-i\hbar)^n\frac{\partial^n}{\partial x^n}$

$\hat x = x$ $\qquad$ $\hat V = V$

$\hat H = \frac{\hat p^2}{2m} + \hat V$ $\qquad$ Hamiltonov operator

naj so $f(z) = \sum_n c_n z^n$ analitične funk.

def: $f(\hat A) = \sum_n c_n \hat A^n$

npr. $e^{\hat A} = 1 + \hat A + \frac{1}{2!}\hat A^2 + \dots + \frac{1}{n!}\hat A^n + \dots$

Komutatorji

operator $\hat A, \hat B, \hat C, \dots$

def. $[\hat A, \hat B] = \hat A\hat B - \hat B\hat A$

Lastnosti:

- $[\lambda\hat A, \hat B] = \lambda[\hat A, \hat B]$ $\qquad \lambda\in\mathbb{C}$
- $[\hat A, \hat B] = -[\hat B, \hat A]$
- $[\hat A\hat B, \hat C] = \hat A[\hat B, \hat C] + [\hat A, \hat C]\hat B$
- $[\hat A, [\hat B, \hat C]] + [\hat B, [\hat C, \hat A]] + [\hat C, [\hat A, \hat B]] = 0$
- Baker-Hausdorffova lema
  $e^{\hat A}\hat B e^{-\hat A} = \hat B + [\hat A, \hat B] + \frac{1}{2!}[\hat A, [\hat A, \hat B]] + \dots + \frac{1}{n!}[\hat A, [\hat A, \dots [\hat A, \hat B]\dots]] + \dots$

Primer $\qquad \hat A = x \qquad \hat B = \hat p = -i\hbar\frac{\partial}{\partial x}$

1D $$[\hat x, \hat p]f(x) = x(-i\hbar)\frac{\partial}{\partial x}f(x) - (-i\hbar)\frac{\partial}{\partial x}x f(x) = -i\hbar\left(x\frac{\partial f}{\partial x} - f - x\frac{\partial f}{\partial x}\right)$$
$$= i\hbar f$$

3D $$[r_\alpha, p_\beta] = \begin{cases} i\hbar & ;\ \alpha = \beta \\ 0 & ;\ \alpha\neq\beta\end{cases} = i\hbar\,\delta_{\alpha\beta}$$

Lastnosti p in H

per partes $\qquad \int u\,dv = uv - \int v\,du$

φ, ψ: $\quad \bullet \displaystyle\int_{-\infty}^{\infty} \varphi \frac{d}{dx}\psi\,dx = \underbrace{\varphi\psi\Big|_{-\infty}^{\infty}}_{=0} - \int \psi \frac{d\varphi}{dx}\,dx = -\int \frac{d\varphi}{dx}\psi\,dx$

za hitro padajoče funkcije

$\hat{A} = \frac{\partial}{\partial x}$ je antisimetričen / antihermitski

$\bullet \displaystyle\int_{-\infty}^{\infty} \varphi \frac{d^2}{dx^2}\psi\,dx \overset{\text{per partes}}{=} -\int_{-\infty}^{\infty} \frac{d\psi}{dx}\frac{d\varphi}{dx}\,dx \overset{\text{per part.}}{=} \int_{-\infty}^{\infty} \psi \frac{d^2\varphi}{dx^2}$

$\hat{A} = \frac{\partial^2}{\partial x^2}$ je simetričen / hermitski

$\bullet \ \hat{A} = \hat{p} = -i\hbar\frac{\partial}{\partial x}$

$$\int_{-\infty}^{\infty} \varphi^* \hat{A}\psi\,dx = \int_{-\infty}^{\infty} \varphi^* \left(-i\hbar\frac{\partial}{\partial x}\right)\psi\,dx = \int_{-\infty}^{\infty} \frac{\partial\varphi^*}{\partial x} i\hbar\,\psi\,dx =$$

$$= \int_{-\infty}^{\infty} \left(-i\hbar\frac{\partial\varphi}{\partial x}\right)^*\psi\,dx = \int_{-\infty}^{\infty} (\hat{p}\varphi)^*\psi\,dx$$

$\int \varphi^* \hat{A}\psi\,dx = \int (\hat{A}\varphi)^*\psi\,dx$ simetričen / hermitski

Ehrenfestov teorem

$\hat{A}, \psi, \langle\hat{A}\rangle \qquad \langle\hat{A}\rangle = \int \psi^*\hat{A}\psi\,dx \qquad\qquad i\hbar\frac{\partial\psi}{\partial t} = H\psi$

$$\frac{d}{dt}\langle\hat{A}\rangle = \int \frac{\partial\psi^*}{\partial t} A\psi + \psi^*\frac{\partial A}{\partial t}\psi + \psi^* A\frac{\partial\psi}{\partial t}\,dx$$

$$= \left\langle\frac{\partial A}{\partial t}\right\rangle + \frac{1}{i\hbar}\int \left(-(H\psi)^* A\psi + \psi^* A(H\psi)\right)dx$$

$$= \left\langle\frac{\partial A}{\partial t}\right\rangle + \frac{1}{i\hbar}\int -\psi^* AH\psi + \psi^* HA\psi\,dx \qquad \text{ker je } H \text{ hermitski}$$

$$\boxed{\frac{d}{dt}\langle A\rangle = \left\langle\frac{\partial A}{\partial t}\right\rangle + \frac{1}{i\hbar}\langle[A,H]\rangle}$$

Primeri:

① $A = x \qquad \frac{d\langle x\rangle}{dt} = 0 + \frac{1}{i\hbar}\left\langle\left[x, \frac{p^2}{2m} + V\right]\right\rangle = \frac{1}{i\hbar}\frac{1}{2m}2i\hbar\langle\hat{p}\rangle = \frac{1}{m}\langle p\rangle$

$[x, p^2] = p\underbrace{[x,p]}_{i\hbar} + \underbrace{[x,p]}_{i\hbar}p = 2i\hbar p$

$[x, V] = 0$

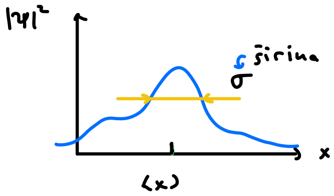
② $\frac{d\langle p\rangle}{dt} = m\frac{d^2\langle x\rangle}{dt^2} = \frac{1}{i\hbar}\langle[\hat{p},\hat{H}]\rangle = \frac{1}{i\hbar}\left\langle\left[p, \frac{p^2}{2m} + V\right]\right\rangle =$

$= \frac{1}{2mi\hbar}\langle\underbrace{[p, p^2]}_{=0}\rangle + \frac{1}{i\hbar}\langle[p, V]\rangle = \ldots$

$[p, V]f = (pV - Vp)f = -i\hbar\frac{\partial}{\partial x}(Vf) + i\hbar V\frac{\partial}{\partial x}f = -i\hbar\cancel{V\frac{\partial}{\partial x}f} - i\hbar\left(\frac{\partial}{\partial x}V\right)f + i\hbar\cancel{V\frac{\partial}{\partial x}f}$

$\ldots = -\frac{1}{i\hbar}i\hbar\left\langle\frac{\partial V}{\partial x}\right\rangle \quad \Rightarrow \quad \boxed{m\frac{d^2\langle x\rangle}{dt^2} = -\left\langle\frac{\partial V}{\partial x}\right\rangle = \langle F\rangle}$ Ehrenfestov teorem

Nedoločenost (širina porazdelitve)



$(\Delta x)^2 = \sigma^2 = \langle x^2\rangle - \langle x\rangle^2 = \langle (x-\langle x\rangle)^2\rangle$

$(\Delta A)^2 = \langle A^2\rangle - \langle A\rangle^2$ $\quad\quad$ $\boxed{\Delta A\, \Delta B \geq \frac{1}{2}|\langle [A,B]\rangle|}$

$(\Delta p)^2 = \langle p^2\rangle - \langle p\rangle^2$ $\quad\quad$ $\boxed{\Delta x\, \Delta p \geq \frac{\hbar}{2}}$ relacija nedoločenosti

širina porazdelitve in ne napaka meritve

Formalizem kvantne mehanike

1. Vektorski prostor, Hilbertov prostor L^2 (v kvadratu integrabilne funkcije)
   - $\psi \in L^2$
   - $\exists$ baza $\{\varphi_n\}$ $\quad n \in \mathbb{N}$ $\quad$ števna baza
     ($\{\varphi_k\}$ $\quad k \in \mathbb{R}$ $\quad$ neštevna baza $\quad$ Banachov prostor)
2. Skalarni produkt
   $\varphi, \psi \in L^2$
   $$(\varphi,\psi) = (\varphi|\psi) = \langle\varphi,\psi\rangle = \langle\varphi|\psi\rangle = \int_{-\infty}^{\infty}\varphi^*\psi\,dx$$
   Lastnosti
   - $\langle\varphi|\psi\rangle = \langle\psi|\varphi\rangle^*$
   - $\langle\psi|\psi\rangle \geq 0$, če $\langle\psi|\psi\rangle = 0 \Rightarrow \psi = 0$
   - $|\langle\varphi|\psi\rangle|^2 \leq \langle\varphi|\varphi\rangle\langle\psi|\psi\rangle$ $\quad\quad$ $(\vec a\cdot\vec b \leq |\vec a||\vec b|)$
3. Ket - stanje sistema (vektor)
   $\psi \in L^2$ $\quad\quad$ $|\psi\rangle \in L^2$
4. Linearni operatorji
   $\hat A\psi = \psi_1$ $\quad\quad$ $\mathcal{D}(A)$ domena (na katere funk. deluje operator)
   $\hat A(\lambda\psi + \mu\varphi) = \lambda\hat A\psi + \mu\hat A\varphi$ $\quad\quad$ $\lambda, \mu \in \mathbb{C}$ $\quad$ linearnost
5. Bra $\quad$ $\langle$bra$|$ket$\rangle$ $\rightarrow$ skalarni produkt
   linearni funkcional (operator ki funk. preslika v število)
   $\psi(x) \in L^2$ $\quad\quad$ $\hat f\psi = z$ $\quad$ $z \in \mathbb{C}$

   Rieszov izrek

   Za vsak lin. funkcional $\hat f\psi = z$ $\quad\exists\quad$ $f_z \in L^2$: $\quad z = \int f_z^*(x)\,\psi(x)\,dx = \langle f_z|\psi\rangle$

   $\hat f\psi = \int f_z^*(x)\,\psi\,dx = \langle \hat f|\psi\rangle$
   $\hat f \ldots = \int f_z^*(x)\ldots dx$
   $\hat f \ldots = \langle f|$
6. Razvoj stanja po dani bazi $\{\varphi_n\}$
   $\{\varphi_n\}$ ortonormirane baze $\quad\quad$ $\int\varphi_n^*\varphi_m\,dx = \delta_{nm}$

   $\psi(x) = \sum_n c_n\varphi_n(x)$ $\quad\quad$ $/\cdot\int\varphi_m^*\,dx$

   $\boxed{\int\varphi_m^*\psi(x)\,dx = c_m}$ $\quad\quad$ $|\psi\rangle = \sum_n |n\rangle\underbrace{\langle n|\psi\rangle}_{c_n}$

   $\psi(x) = \sum_n\left(\int_{-\infty}^{\infty}\varphi_n^* \ldots dx\right)\varphi_n(x)\,\psi$ $\quad\quad$ $\psi = \sum_n\varphi_n\int\varphi_n^*(x')\,\psi\,dx'$

„po Diracu" $\{|\varphi_n\rangle\} = \{|n\rangle\}$ $\boxed{|\varphi_n\rangle = |n\rangle}$

$|\psi\rangle = \sum_n c_n |n\rangle \quad /\cdot\langle m|$

$\langle m|\psi\rangle = \sum_n c_n \langle m|n\rangle = c_m$

$$|\psi\rangle = \sum_n \langle n|\psi\rangle|n\rangle = \sum_n |n\rangle\langle n|\psi\rangle = \Big(\sum_n |n\rangle\langle n|\Big)|\psi\rangle = I|\psi\rangle$$

$\boxed{I = \sum_n |n\rangle\langle n|}$ identiteta

7) Zapis operatorja v dani bazi

$\{|n\rangle\}$ $\hat A|\psi\rangle = |\psi_1\rangle$ $\langle m|n\rangle = \delta_{nm}$

$$\hat A|\psi\rangle = I\hat A I|\psi\rangle = \sum_m |m\rangle\langle m|A\sum_n |n\rangle\langle n|\psi\rangle = \sum_{m,n}|m\rangle A_{mn}\langle n|,$$

vrinemo kompleten sistem

$A_{mn} = \langle m|\hat A|n\rangle$

matrični element

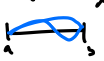
$$\hat A = \sum_{m,n}|m\rangle A_{mn}\langle n|$$

Naj bo $|\psi\rangle = \sum c_n|n\rangle$ $|\psi_1\rangle = \sum_n d_n|n\rangle$

$$\hat A|\psi\rangle = \sum_{mn}|m\rangle A_{mn}\underbrace{\langle n|\sum_k c_k|k\rangle}_{c_n} = \sum_{mn}|m\rangle A_{mn}c_n = \underbrace{\sum_m d_m|m\rangle}_{|\psi_1\rangle} =$$

$$= \sum_m\Big(\sum_n A_{mn}c_n\Big)|m\rangle$$

Primer: $\hat A = \hat p = -i\hbar\frac{\partial}{\partial x}$ naj bodo bazni vektorji: $\varphi_n(x) = c_n \sin k_n x$, $|n\rangle$



$\hat p\,\psi(x) = -i\hbar\frac{\partial}{\partial x}\psi(x)$

$$A_{mn} = \int_a^b c_m^* c_n \sin k_m x\,(i\hbar)\frac{\partial}{\partial x}\sin k_n x\,dx \quad ✓$$

$\psi = \sum_n c_n\varphi_n$ $c_n = \int \varphi_n^*\psi\,dx$

$d_m = \sum_n A_{mn}c_n \Rightarrow \sum d_m\varphi = \hat A\psi$ z matrič. el. lahko izračunamo člene razvoja $\hat A\psi$.

8) Hermitski ali simetrični operatorji:

$\langle\varphi|\hat A|\psi\rangle = \langle\varphi|\hat A\psi\rangle = \langle\hat A\varphi|\psi\rangle$ Simetričen (npr. gibalne količine $\hat p$)

Lastnosti sim. operatorjev: $\hat A \to A$ brez strešice

- $A|\psi\rangle = a|\psi\rangle \quad /\cdot\langle\psi|$ iščemo lastne vrednosti

$\langle\psi|A|\psi\rangle = a\langle\psi|\psi\rangle$

$\langle A\psi|\psi\rangle = \langle\psi|A\psi\rangle = a\langle\psi|\psi\rangle \in \mathbb{R}$ ker je sim.

$\Leftrightarrow a \in \mathbb{R}$

če je A simetričen ima realne lastne vrednosti

- $A|\psi\rangle = a|\psi\rangle \quad /\cdot\langle\varphi|$

$A|\varphi\rangle = b|\varphi\rangle \quad /\cdot\langle\psi|$

- $\langle \varphi | A | \psi \rangle = a \langle \varphi | \psi \rangle$

$\langle \psi | A | \varphi \rangle = b \langle \psi | \varphi \rangle \qquad /^*$

$\langle \psi | A | \varphi \rangle^* = b \langle \varphi | \psi \rangle$

$\langle \psi | A | \varphi \rangle^* = \langle \psi | A \varphi \rangle^* = \langle A\varphi, \psi \rangle \overset{\text{sim.}}{=} \langle \varphi | A \psi \rangle = \langle \varphi | A | \psi \rangle$

- $\langle \varphi | A | \psi \rangle = b \langle \varphi, \psi \rangle$

$-$

$0 = (a-b) \langle \varphi | \psi \rangle \Rightarrow$ če $a \neq b$ je $\langle \varphi, \psi \rangle = 0 \Leftrightarrow \varphi \perp \psi$

9 Hermitsko adjungirani operator

$A, \quad |\varphi\rangle, \ |\psi\rangle$

$B: \quad \langle \varphi | A | \psi \rangle = \langle B\varphi, \psi \rangle \qquad B = A^\dagger \qquad \dagger \ldots$ bodalo, dagger

$(B = A^\dagger$ mat zapis, adjungacija$)$

Lastnosti:

- $A = zB$

$\langle \varphi | A | \psi \rangle = \langle \varphi | zB | \psi \rangle = z \langle \varphi | B | \psi \rangle = z \langle B^\dagger \varphi | \psi \rangle = z \langle \psi | B^\dagger | \varphi \rangle^* =$

$= \langle z^* B^\dagger \varphi | \psi \rangle$

$\langle A^\dagger \varphi | \psi \rangle \quad \Rightarrow A^\dagger = z^* B^\dagger$

$A = zI \Rightarrow A^\dagger = z^* \qquad A = x \Rightarrow A^\dagger = x$

- $A = |m\rangle\langle n|$

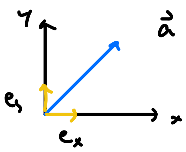
$\langle \varphi | A | \psi \rangle = \langle \varphi | m \rangle \langle n | \psi \rangle = (\langle \psi | n \rangle \langle m | \varphi \rangle)^* = \langle A^\dagger \varphi | \psi \rangle$

$\Rightarrow A^\dagger = |n\rangle\langle m|$

- $(\mu A + \lambda B)^\dagger = \mu^* A^\dagger + \lambda^* B^\dagger$
- $(AB)^\dagger = B^\dagger A^\dagger$

$\langle \varphi | AB | \psi \rangle = \langle A^\dagger \varphi | B \psi \rangle = \langle B^\dagger A^\dagger \varphi | \psi \rangle$

- Projektor



$\vec{a} = (\vec{e}_x \cdot \vec{a}) \vec{e}_x + (\vec{e}_y \cdot \vec{a}) \vec{e}_y$

$P_x \qquad P_y$

$P_n = |n\rangle\langle n|$

idepotentni operator

$P_n^2 = P_n P_n = |n\rangle\langle n|n\rangle\langle n| = P_n$

$I = \sum_n P_n$

10 Kako najdemo $A^\dagger$, če poznamo A?

$A = \sum_{mn} |m\rangle A_{mn} \langle n| \qquad A^\dagger = \sum_{mn} |n\rangle A_{mn}^* \langle m| \overset{\substack{m \to n \\ n \to m}}{=} \sum_{nm} |m\rangle A_{nm}^* \langle n|$

$(\hat{A})_{mn} = A_{mn} \qquad (\hat{A}^\dagger)_{mn} = A_{nm}^*$

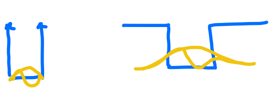
11 Sebi adjungirani operatorji (hermitski)

naj velja: ⓐ $\langle \varphi | A | \psi \rangle = \langle A\varphi | \psi \rangle$ hermitski ali simetrični

ⓑ $A = A^\dagger \quad \Leftarrow$ Sebi adjungirani če velja ⓐ in $D(A) = D(A^\dagger)$

$\Rightarrow \exists \{|n\rangle\}, \quad A|n\rangle = a|n\rangle$

Primer



ⓒ $\hat{A} = \hat{p} = -i\hbar \frac{\partial}{\partial x}$

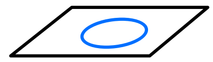
$-i\hbar \frac{\partial}{\partial x} \varphi(x) = \lambda \varphi(x)$

$\Rightarrow \varphi(x) = C e^{i \frac{\lambda}{\hbar} x}$

Robni pogoji: $\Rightarrow C = 0$

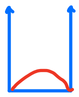
$$\hat H = \frac{\hat p^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \Rightarrow C_2\, e^{\pm i\frac{\lambda}{\hbar}x}$$ lahko razumemo v smislu.

ⓑ Periodični robni pogoji:



$$\varphi(s+2\pi) = \varphi(s)$$
$$e^{i\frac{\lambda}{\hbar}(u+2\pi)} = e^{i\frac{\lambda}{\hbar}u}$$
$$\lambda_n \in \mathbb{R}$$

ⓒ



Izračunaj

$$\psi = c(a^2-x^2)$$

$$H = \frac{p^2}{2m}$$

$$\langle H\rangle = \langle E\rangle = \int c^2(a^2-x^2)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)(a^2-x^2)\,dx > 0$$

Kakšna je nedoločenost E (ΔE)?

$$(\Delta E)^2 = \langle H^2\rangle - \langle H\rangle^2 < 0 \quad ???$$

$$\langle H^2\rangle = \int c^2(a^2-x^2)\left(\frac{\hbar^4}{4m^2}\frac{\partial^4}{\partial x^4}\right)(a^2-x^2)\,dx = 0$$

⑫ Unitarni operatorji: ("rotacije")

U^{-1} inverzni

$$U^{-1}U = UU^{-1} = I$$

unitarni op. so tisti $U^{-1} = U^+$ $\qquad UU^+ = U^+U = I$

Lastnosti:

- $\langle \varphi|\psi\rangle = \langle U^+\tilde\varphi|U^+\tilde\psi\rangle = \langle\tilde\varphi|UU^+|\tilde\psi\rangle = \langle\tilde\varphi|\tilde\psi\rangle$

  $U|\varphi\rangle = |\tilde\varphi\rangle \qquad |\varphi\rangle = U^+|\tilde\varphi\rangle$

  $U|\psi\rangle = |\tilde\psi\rangle \qquad |\psi\rangle = U^+|\tilde\psi\rangle$

  Skalarni produkt se ohranja.
- $\langle\varphi|A|\psi\rangle = \langle U^+\tilde\varphi|A|U^+\tilde\psi\rangle = \langle\tilde\varphi|UAU^+|\tilde\psi\rangle = \langle\tilde\varphi|\tilde A|\tilde\psi\rangle$

  $\tilde A = UAU^+$
- $A = \mu B + \lambda CD \qquad \tilde B = UBU^+$

  $\tilde A = \mu\tilde B + \lambda\tilde C\tilde D$
- Če velja $K = K^+ \Rightarrow U = e^{iK}$ je unitaren
  - $UU^+ = e^{iK}e^{-iK} = I$
  - Enoparametričen unitaren operator

    $U(s)$: $\exists\, K = K^+$, $U(s) = e^{isK}$

⑬ Časovni razvoj kvantnega stanja

- Stacionarna stanja, $H \neq H(t)$

  $$H = \frac{p^2}{2m} + V(\vec r)$$

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi \qquad \Psi(\vec r,t) = \psi(\vec r)\,f(t)$$

$$i\hbar\,\psi\frac{\partial f}{\partial t} = H\psi f \qquad /:\psi f$$

$$\underbrace{\frac{i\hbar}{f}\frac{\partial f}{\partial t}}_{\text{od } t} = \underbrace{\frac{1}{\psi}H\psi}_{\text{od } x} = E \quad = \text{konst.}$$

$$\Rightarrow \boxed{\Psi(\vec r,t) = \psi(\vec r)\,e^{-i\frac{E}{\hbar}t}} \qquad |\Psi|^2 = |\psi|^2$$

- $H|\varphi_n\rangle = E_n|\varphi_n\rangle$

$$|\psi(t)\rangle\Big|_{t=0} = \sum_n |\varphi_n\rangle\langle\varphi_n|\psi(0)\rangle = \sum_n \langle\varphi_n|\psi(0)\rangle\,|\varphi_n\rangle$$

$\hookrightarrow \varphi_n(\vec r)$

$$|\psi(t)\rangle = \sum_n \langle\varphi_n|\psi(0)\rangle\, e^{-i\frac{E}{\hbar}t}\,|\varphi_n\rangle$$

$$\psi(\vec r,t) = \sum_n c_n\, e^{-i\frac{E_n}{\hbar}t}\,\varphi_n(\vec r)$$

$$\hat f(\hat A) = \sum c_n \hat A^n \qquad \hat A|n\rangle = a_n|n\rangle$$

$$f(\hat A)|\psi\rangle = \sum_n c_n f(a_n)|\psi\rangle$$

$$e^{-i\frac{E}{\hbar}t}\varphi_n(\vec r) = e^{-i\frac{\hat H}{\hbar}t}\varphi_n(\vec r)$$

$\hookrightarrow I - \frac{iE_n}{\hbar}t + \frac{1}{2!}\left(\frac{iE_n}{\hbar}\right)^2 t^2 + \mathcal{O}(t^3)$

$$\psi(\vec r,t) = e^{-i\frac{Ht}{\hbar}}\sum_n c_n\varphi_n(\vec r) = e^{-i\frac{Ht}{\hbar}}\psi(\vec r,0)$$

$$U(t_1,t_2) = e^{-\frac{iH}{\hbar}(t_2-t_1)}$$

! $\psi(\vec r,t_2) = U(t_2,t_1)\,\psi(\vec r,t_1) \qquad U = e^{iu}$

Naj bo $\delta\psi(\vec r,t) = \psi(\vec r,t+dt) - \psi(\vec r,t) = U(t+dt,t)\psi(\vec r,t) - \psi(\vec r,t) \qquad U(t) = e^{-\frac{iHt}{\hbar}}$

$dt \ll 1 \Rightarrow$ razvoj $\Rightarrow \quad \delta\psi = \left(1 - i\frac{H}{\hbar}dt + \mathcal{O}(dt^2)\right)\psi(\vec r,t) \qquad /:dt$

$$\frac{d\psi}{dt} = -i\frac{H}{\hbar}\psi \Rightarrow i\hbar\frac{\partial}{\partial t}\psi = H\psi \quad \text{Schrödingerjeva en.}$$

(14) Reprezentacija p in x

- $f(x) = \int_{-\infty}^{\infty}\hat f(k)\,e^{ikx}\,dk, \qquad \hat f(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} f(x)\,e^{-ikx}\,dx$

Vstavimo eno v drugo $\quad f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x')\,\underbrace{e^{-ikx'+ikx}}_{\delta(x-x')}\,dx'\,dk = \int_{-\infty}^{\infty}\delta(x-x')\,f(x')\,dx'$

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}\,dk \qquad \text{funkcija delta (ni funkcija)}$$

- Prosti delec : $V(x) = 0$

$i\hbar\frac{d}{dt}|\psi\rangle = \frac{\hat p^2}{2m}|\psi\rangle, \qquad |\psi\rangle \to |\varphi_p\rangle = |p\rangle$ lastna stanja

$\hat p|\varphi_p\rangle = p|\varphi_p\rangle, \qquad p \in \mathbb{R}$

$-i\hbar\frac{\partial}{\partial x}\varphi_{p_0}(x) = p_0\,\varphi_{p_0}(x) \Rightarrow \varphi_{p_0}(x) = c\,e^{i\frac{p_0}{\hbar}x} = \frac{1}{\sqrt{2\pi\hbar}}e^{i\frac{p_0}{\hbar}x} \qquad k = \frac{p}{\hbar}$

$\int_{-\infty}^{\infty}\varphi_{p_0}^*(x)\,\varphi_p(x)\,dx = \delta(p-p_0) \quad ; \quad c = \frac{1}{\sqrt{2\pi\hbar}}$

$|p_0\rangle = |\varphi_{p_0}\rangle \qquad \langle\varphi_{p_0}|\varphi_p\rangle = \delta(p-p_0)$

Lastnosti:

$\delta(ax) = \frac{1}{|a|}\delta(x)$

$$\psi(x) = \int \tilde{\psi}(p)\, \varphi_p(x)\, dp$$
$$\tilde{\psi}(p) = \int \psi(x)\, \varphi_p^*(x)\, dx$$

Parsevalova enačba $\qquad \int |\psi|^2 dx = \int |\tilde{\psi}|^2 dp$

- Karakteristična funkcija

$$\hat{p}\,\psi(x) = -i\hbar \frac{\partial}{\partial x}\psi(x) = \int \tilde{\varphi}(p) \underbrace{\left(-i\hbar \frac{\partial}{\partial x} \varphi_p(x)\right)}_{p\cdot \varphi_p(x)} dp = \int \left(p\,\tilde{\psi}(p)\right) \varphi_p(x)\, dx$$

Vsako odvajanje preide na množenje

$$\left(-i\hbar \frac{\partial}{\partial x}\right)^{(n)} \psi(x) \leftrightarrow p^n\, \tilde{\psi}(p)$$

$$\hat{x}\,\psi(x) = x\,\psi(x) = \int \tilde{\varphi}(p)\, x\, \varphi_p(x)\, dp = \int \tilde{\varphi}(p) \frac{\partial}{\partial p} \varphi_p\, dp = \int \left(i\hbar \frac{\partial}{\partial p} \tilde{\varphi}(p)\right) \varphi_p(x)\, dp$$

$$x^n\, \psi(x) \leftrightarrow \left(i\hbar \frac{\partial}{\partial p}\right)^{(n)} \tilde{\psi}(p)$$

- Lastne stanje $\hat{x}$

$$\hat{x}\,\psi_0(x) = x\,\psi_0(x) = x_0\,\psi_0(x)$$
lastna vrednost

$$x \int \tilde{\varphi}_0(p)\, \varphi_p(x)\, dp = \int \tilde{\varphi}_0(p)\, x\, \varphi_p(x)\, dp = \int \left(i\hbar \frac{\partial}{\partial p} \tilde{\varphi}_0(p)\right) \varphi_p(x)\, dx$$

$$i\hbar \frac{\partial}{\partial p} \tilde{\varphi}_0(p) = x_0\, \tilde{\varphi}_0(p) \Rightarrow \tilde{\varphi}_0(p) = \frac{1}{\sqrt{2\pi\hbar}} e^{-i\frac{p}{\hbar}x_0}$$

$$\psi_0(x) = \int \varphi_p^*(x)\, \varphi_p(x)\, dp = \delta(x - x_0)$$

15 Verjetnostni amplitudi $\langle p|\psi\rangle$ in $\langle x|\psi\rangle$

$\psi(x) \in \mathbb{C}$

$\quad\; \in L^2$

$|\psi\rangle \in L^2 \qquad \psi(x)$ ali $\tilde{\psi}(p)$ ali c_n

- Naj bo $\quad |\psi\rangle = \int \tilde{\psi}(p)\, |p\rangle\, dp \qquad / \langle p_1|$

$$\langle p_1|\psi\rangle = \int \tilde{\psi}(p) \underbrace{\langle p_1|p\rangle}_{\delta(p-p_1)} dp = \int \tilde{\psi}(p)\, \delta(p - p_1)\, dp = \tilde{\psi}(p_1)$$

$$\Rightarrow \quad \boxed{\tilde{\psi}(p) = \langle p|\psi\rangle} \quad \in \mathbb{C}$$

- Komentar (enako kot ↑ le v števni bazi

$|\psi\rangle = \sum_n c_n\, |n\rangle \qquad / \cdot \langle n_1|$

$\langle n_1|\psi\rangle = c_{n_1}$

$c_n = \langle n|\psi\rangle \qquad \in \mathbb{C}$

- $|\psi\rangle = \int \tilde{\psi}(p)\, |p\rangle\, dp \qquad / \langle x_0| \qquad\qquad x|x_0\rangle = x_0|x_0\rangle$

$$\langle x_0|\psi\rangle = \int \tilde{\psi}(p) \underbrace{\langle x_0|p\rangle}_{\varphi_p(x_0)} dp = \psi(x_0)$$

$$\boxed{\psi(x) = \langle x | \psi \rangle}$$ razvoj po zveznem spektru

- $I = \sum_n |n\rangle\langle n|$

$|\psi\rangle = \sum_n |n\rangle \underbrace{\langle n|\psi\rangle}_{c_n} = \sum_n c_n |n\rangle$

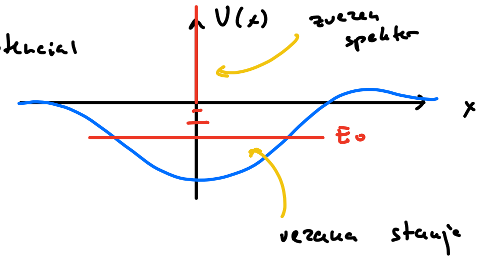
$I = \int |p\rangle\langle p| \, dp$

$|\psi\rangle = I|\psi\rangle = \int |p\rangle\langle p|\psi\rangle \, dp = \int |p\rangle \, \tilde{\psi}(p) \, dp$

$I = \int |x\rangle\langle x| \, dx$

$|\psi\rangle = \int |x\rangle\langle x|\psi\rangle \, dx = \int \psi(x) |x\rangle \, dx$

- potencial



Vezano stanje obstaja le če je $\int V < 0$

$$I = \sum_n |E_n\rangle\langle E_n| + \int |E\rangle\langle E| \, dE$$

(16) Kompleten sistem med seboj komutirajočih operatorjev

A, B, $[A, B] = 0 \iff \exists \{|n\rangle\} : A|n\rangle = a_n|n\rangle$ in $B|n\rangle = b_n|n\rangle$

Primer

- $H = \frac{p^2}{2m} = A$

  $p = B$

- H-atom

  $V \propto \frac{1}{r}$ $\quad H, \vec{L}, L_z, \vec{S}, S_z$

  $\Rightarrow |\psi\rangle = |n, l, m_l, s, m_s\rangle$

(17) Postulati kvantne mehanike

Kopenhagenska interpretacija

1. Svet delimo na kvantnega in klasičnega
2. Vsaka opazljivka je hermitski operator $A = A^\dagger$
3. Pričakovana vrednost so $\langle\psi|A|\psi\rangle \in \mathbb{R}$
4. Dinamika, časovni razvoj

   $i\hbar \frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle$ $\qquad |\psi(t)\rangle = U(t,0)|\psi(0)\rangle$
5. O meritvi

   Pri posamezni meritvi količine A je rezultat ena od lastnih vrednosti enačbe $A|a\rangle = a|a\rangle$

   Verjetnost, da izmerimo ravno „a" je podana z

   $$P_a = |c_a|^2 \qquad c_a = \langle a|\psi\rangle$$

   - Števna baza $|\psi\rangle = \sum_n c_n|n\rangle$ $\qquad P_n = |c_n|^2$
   - Neskončna baza $|\psi\rangle = \int \psi(x)|x\rangle \, dx$ $\qquad |\psi|^2 = g(x)$

Kolaps valovne funkcije

Po izvedeni meritvi, je kvantni sistem v stanju $|a\rangle$

$|\psi\rangle \to |a\rangle$ $\qquad$ neunitarno

↳ kolaps

Ravno

$\hat{p}\,|p_0\rangle = p_0\,|p_0\rangle$

$\hat{x}\,|x_0\rangle = x_0\,|x_0\rangle$

lastno stanje koordinate

$|\psi\rangle = \int |x\rangle\langle x|\psi\rangle\,dx = \int \psi(x)\,|x\rangle\,dx$

po meritvi $\longrightarrow$ $|x_0\rangle$, x_0, $|\psi(x_0)|^2 dx = dP$

$|\psi\rangle = \int |p\rangle\langle p|\psi\rangle\,dp = \int \tilde{\psi}(p)\,|p\rangle\,dp$

$\longrightarrow |\tilde{\psi}(p)|^2 dp = dP$

Verjetnost da najdemo delec z dano gib. kol.

$\langle x|p\rangle = \varphi_p(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{i\frac{p}{\hbar}x}$ lastno stanje operatorja $\hat{p}$

projekcija p na x

$\langle x|x_0\rangle = \delta(x-x_0)$ lastno stanje operatorja $\hat{x}$

nista normalizabilni zato sta kvazi vektorja

$|x_0\rangle = \int \underbrace{\delta(x-x_0)}\,|x\rangle\,dx$

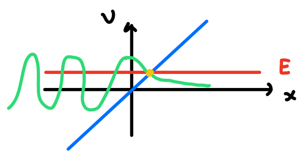
ekvivalentno cn pri diskretnih stanjih

$\langle x_1|x_0\rangle = \int \delta(x-x_0)\langle x_1|x\rangle\,dx = \int \delta(x-x_0)\,\delta(x-x_1)\,dx = \delta(x_1-x_0)$

$\int(\delta(x-x_1))^2dx = \times$

Prosti pad

$\frac{p^2}{2m}\psi + mgx\,\psi = E\,\psi$



$\psi(x) = \int \tilde{\psi}(p)\,\frac{e^{i\frac{p}{\hbar}x}}{\sqrt{2\pi\hbar}}\,dp$

Airyjeva funkcija

$y'' - x\,y = 0$

$Ai(x) = \frac{1}{\pi}\int_0^\infty \cos\left(\frac{k^3}{3} + kx\right)dx$

prehod na p (Fourier)

$\frac{\hat{p}^2}{2m}|\psi\rangle + V(x)\,|\psi\rangle = E\,|\psi\rangle$

$\frac{p^2}{2m}|\tilde{\psi}\rangle + mg\left(i\hbar\frac{\partial}{\partial p}\right)|\tilde{\psi}\rangle = E\,|\tilde{\psi}\rangle$ DE 1. reda

$\Rightarrow\quad |\tilde{\psi}\rangle = Ce^{i\left(\frac{p^3}{6} + mEp\right)/(\hbar g m^2)}$

Harmonski oscilator

$H = E = \frac{p^2}{2m} + \frac{1}{2}kx^2$, $\ddot{x} + \omega^2 x = 0$ $\omega^2 = \frac{k}{m}$ Klasičen primer

$x = x_0\cos(\omega t - \delta)$

Kvantni primer

$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2x^2 = \frac{1}{2}\hbar\omega\left(\frac{x^2}{\xi^2} - \xi^2\frac{d^2}{dx^2}\right) =$ $\xi^2 = \frac{\hbar}{m\omega}$

$= \frac{1}{4}\hbar\omega\left(\left(\frac{x}{\xi} + \xi\frac{d}{dx}\right)\left(\frac{x}{\xi} - \xi\frac{d}{dx}\right) + \left(\frac{x}{\xi} - \xi\frac{d}{dx}\right)\left(\frac{x}{\xi} + \xi\frac{d}{dx}\right)\right) = \ldots$

$$\boxed{\begin{aligned} a &= \frac{1}{\sqrt{2}}\left(\frac{x}{\xi} + \xi\frac{d}{dx}\right) = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{i}{m\omega}p\right) \\ a^\dagger &= \frac{1}{\sqrt{2}}\left(\frac{x}{\xi} - \xi\frac{d}{dx}\right) = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{i}{m\omega}p\right)\end{aligned}}$$

Anihilacijski operator

Kreacijski operator

$$x = \frac{s}{\sqrt{2}}(a + a^{+})$$

$$\frac{d}{dx} = \frac{1}{s\sqrt{2}}(a - a^{+})$$

$$[a, a^{+}] = \frac{1}{\sqrt{2}}\left(\frac{x}{s} + s\frac{d}{dx}\right)\frac{1}{\sqrt{2}}\left(\frac{x}{s} - s\frac{d}{dx}\right) - \frac{1}{\sqrt{2}}\left(\frac{x}{s} - s\frac{d}{dx}\right)\frac{1}{\sqrt{2}}\left(\frac{x}{s} + s\frac{d}{dx}\right)$$

$$= \frac{1}{2}\left(\frac{x^2}{s^2} - x\frac{d}{x} + \frac{d}{dx}x - s^2\frac{d^2}{dx^2} - \left(\frac{x^2}{s^2} + x\frac{d}{dx} - \frac{d}{dx}x - s^2\frac{d^2}{dx^2}\right)\right)$$

$$= \frac{d}{dx}x - x\frac{d}{dx} = \left[\frac{d}{dx}, x\right] = -\left[x, -i\hbar\frac{d}{dx}\right]\frac{-1}{i\hbar} = \frac{i\hbar}{i\hbar} = 1$$

$$\dots = \frac{1}{2}\hbar\omega\left(\underbrace{aa^{+}}_{a^{+}a+1} + a^{+}a\right) =$$

$$\left[x, -i\hbar\frac{d}{dx}\right] = i\hbar \qquad \boxed{[a, a^{+}] = 1}$$

$$\boxed{H = \hbar\omega\left(a^{+}a + \frac{1}{2}\right)}$$

Operator broja (number operator)

$\hat{n} = a^{+}a$ $\qquad \hat{n}^{+} = a^{+}a = \hat{n}$ $\qquad$ hermitski

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

$$\hat{n}|\varphi_\lambda\rangle = \lambda|\varphi_\lambda\rangle \qquad /\cdot\langle\varphi_\lambda|$$

$$\langle\varphi_\lambda|\hat{n}|\varphi_\lambda\rangle = \langle\varphi_\lambda|a^{+}a|\varphi_\lambda\rangle = \underbrace{\langle a\varphi_\lambda|a\varphi_\lambda\rangle}_{\geq 0} = \underbrace{\lambda}_{\geq 0}\underbrace{\langle\varphi_\lambda|\varphi_\lambda\rangle}_{\geq 0}$$

- Ali je $\lambda = 0$ rješenje?

$$a^{+}a|\varphi_0\rangle = 0$$

$$a|\varphi_0\rangle = 0 \qquad \langle x|\varphi_0\rangle = \varphi_0(x)$$

$$\left(\frac{x}{s} + s\frac{d}{dx}\right)\varphi_0(x) = 0 \quad \Rightarrow \quad \varphi_0(x) = \frac{1}{\sqrt{\sqrt{\pi}\,s}}e^{-\frac{1}{2}\frac{x^2}{s^2}}$$

$\lambda = 0$ je rješenje.

- $$[\hat{n}, a^{+}] = [a^{+}a, a^{+}] = a^{+}\underbrace{[a, a^{+}]}_{1} + \underbrace{[a^{+}, a^{+}]}_{0}a = a^{+} \qquad \boxed{[\hat{n}, a^{+}] = a^{+}}$$

$$[\hat{n}, a] = [a^{+}a, a] = a^{+}[a, a] + [a^{+}, a]a = -a \qquad \boxed{[\hat{n}, a] = -a}$$

- Neka je $|\varphi_\lambda\rangle$ rješenje $\hat{n}|\varphi_\lambda\rangle = \lambda|\varphi_\lambda\rangle$

$$\hat{n}a^{+}|\varphi_\lambda\rangle = (a^{+}\hat{n} + a^{+})|\varphi_\lambda\rangle = (\lambda+1)\underbrace{a^{+}|\varphi_\lambda\rangle}_{c_\lambda|\varphi_{\lambda+1}\rangle} \quad \Rightarrow \quad \lambda = 0, 1, 2, \dots$$

Nova lista vrijednost

$$\langle a^{+}\varphi_\lambda|a^{+}\varphi_\lambda\rangle = c_\lambda^2\langle\varphi_{\lambda+1}|\varphi_{\lambda+1}\rangle = \langle\varphi_\lambda|aa^{+}|\varphi_\lambda\rangle$$

$$c_\lambda = \lambda + 1$$

kreira novo stanje

! $$|\varphi_{n+1}\rangle = \frac{1}{\sqrt{n+1}}a^{+}|\varphi_n\rangle = \dots$$

$\hookrightarrow \frac{1}{\sqrt{n}}a^{+}|\varphi_{n-1}\rangle$

$\hookrightarrow \dots$

$$\boxed{|\varphi_n\rangle = \frac{(a^{+})^n}{\sqrt{n!}}|\varphi_0\rangle} \qquad |n\rangle = \frac{(a^{+})^n}{\sqrt{n!}}|0\rangle$$

$$\langle x|\varphi_n\rangle = \varphi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{x}{s} - s\frac{d}{dx}\right)^n\varphi_0(x)$$

• Ali so $n=0,1,\dots$ vse rešitve?

$$[\hat n, a] = a$$

$$\hat n\, a|n\rangle = (a\hat n - a)|n\rangle = (n-1)\underbrace{a|n\rangle}_{\alpha|n-1\rangle}$$

$$\boxed{\frac{a^n}{\sqrt{(n+1)!}}|\varphi_n\rangle = |\varphi_0\rangle}$$

$\lambda = 7{,}2$? $\qquad \lambda = n+\nu \quad 0<\nu<1$

$$\hat n|\varphi_\lambda\rangle = \lambda|\varphi_\lambda\rangle = (n+\nu)|\varphi_\lambda\rangle$$
$$\hat n a|\varphi_\lambda\rangle = (n-1+\nu)\, a|\varphi_\lambda\rangle$$
$$\hat n a^2|\varphi_\lambda\rangle = (n-2+\nu)\, a^2|\varphi_\lambda\rangle$$
$$\vdots$$
$$\hat n a^n|\varphi_\lambda\rangle = (n-n+\nu)\, a^n|\varphi_\lambda\rangle$$
$$\hat n a^{n+1}|\varphi_\lambda\rangle = \underbrace{(\nu-1)}_{<0}\, a^{n+1}|\varphi_\lambda\rangle \quad \times \quad \Rightarrow \quad \nu = 0$$

$\Rightarrow$
$$H = \hbar\omega\left(\hat n + \tfrac{1}{2}\right)$$
$$E_n = \hbar\omega\left(n+\tfrac{1}{2}\right) \qquad n = 0,1,2,\dots$$

Posplošitve na višje dimenzije

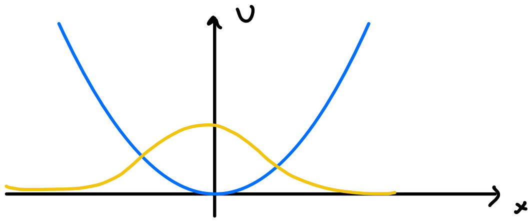
$x_\alpha \qquad \alpha = 1,2,3$

$-i\hbar\frac{d}{dx_\alpha} = p_\alpha$

$$H = \sum_{\alpha=1}^{N}\frac{p_\alpha^2}{2m_\alpha} + \frac{1}{2}\underbrace{k_\alpha}_{m_\alpha\omega_\alpha^2} x_\alpha^2 = \sum_\alpha \hbar\omega_\alpha\left(\hat n_\alpha + \tfrac{1}{2}\right)$$

$$[a_\alpha, a_\beta^\dagger] = \delta_{\alpha\beta}$$

Koherentno stanje



Gauss se premika levo in desno

$$\Psi_n(x,t) = \psi_n(x)\, e^{-i\frac{E_n}{\hbar}t}$$

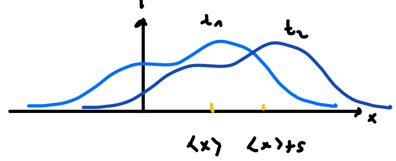
$$a|\varphi_\alpha\rangle = \alpha|\varphi_\alpha\rangle \qquad \alpha = e^{i\delta}|\alpha|$$

Prej smo iskali $\alpha = 0$

Rešitev je premaknjen Gauss

Simetrije

• translacije (premik)



$$U(s)\,\psi(x) = \psi(x-s) = \psi(x) - s\frac{d}{dx}\psi + \frac{s^2}{2!}\frac{d^2}{dx^2}\psi + \dots$$

$$= \left(1 - s\frac{d}{dx} + \frac{s^2}{2!}\frac{d^2}{dx^2}\dots\right)\psi(x) = e^{-s\frac{d}{dx}}\psi(x)$$

$$U(s) = e^{-s\frac{d}{dx}} = e^{-\frac{is}{\hbar}p}$$ (Unitarni) operator premika

$$U(\vec s) = e^{-i\frac{\vec s\cdot\vec p}{\hbar}} = e^{iK}$$ v več dim.

$\hat{\vec p}$ ... generator transformacije

Vaje Baker-Hausdorff

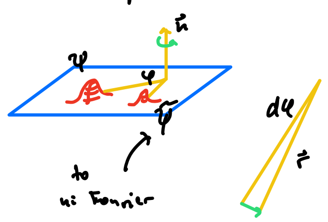
$$\tilde{x} = e^{i\frac{sp}{\hbar}} x \, e^{-i\frac{sp}{\hbar}} = x + \underbrace{[i\tfrac{sp}{\hbar}, x]}_{s} + \frac{1}{2!}\underbrace{[i\tfrac{sp}{\hbar}, \overbrace{[i\tfrac{sp}{\hbar}, x]}^{\text{konst}}]}_{0} + \underbrace{\ldots}_{0}$$

$$\tilde{x} = x + s$$

$$\langle x \rangle = \langle \psi(x-s) | x | \psi(x-s) \rangle = \langle U\psi | x | U\psi \rangle = \langle \psi | U^\dagger x U | \psi \rangle = \langle \psi | \tilde{x} | \psi \rangle =$$
$$= \langle x \rangle |_{s=0} + s$$

• Rotacija

$$\vec{\varphi} = \varphi \vec{n}$$



$d\vec{r}$ translacija $d\vec{r} = d\varphi\, \vec{n} \times \vec{r}$

$$\tilde{\psi}(\vec{r}) = \psi(\vec{r} - d\vec{r}) = \left(I - i d\varphi \frac{(\vec{n}\times\vec{r})}{\hbar} \vec{p} + \mathcal{O}(d\varphi^2) \right) \psi(\vec{r})$$

$$U(\varphi) = \lim_{N\to\infty} \left(I - i \frac{\varphi}{N} \frac{(\vec{n}\times\vec{r})\vec{p}}{\hbar} \right)^N = e^{-\frac{i\varphi \, \vec{n}\vec{L}}{\hbar}}$$

$$(\vec{n}\times\vec{r})\vec{p} = \vec{n}(\vec{r}\times\vec{p}) = \vec{n}\vec{L}$$

$$\boxed{U(\varphi) = e^{-\frac{i\varphi}{\hbar}\vec{n}\vec{L}} \qquad \vec{L} = \vec{r}\times\vec{p}}$$

• Inverzija prostora (parnost)

$$P f(\vec{r}) = f(-\vec{r}) \;, \quad \vec{r} \to -\vec{r}$$

P: $\vec{r} \to -\vec{r}$

$\nabla \to -\nabla$

$\nabla^2 \to \nabla^2$ kin. en. se ne spremeni

$V(\vec{r}) \to ?$ odvisno od potenciala

Naj velja $V(\vec{r}) = V(-\vec{r})$ soda funkcija

Stacionarno stanje $H\psi(x) = E\psi(x)$

$$PH\psi(x) = HP\psi(x) = EP\psi(x)$$

Če je ψ rešitev je tudi $P\psi$

$\Rightarrow$ Dobimo dve novi funkciji

$$\psi_\pm(\vec{r}) = \frac{1}{\sqrt{2}}\left(\psi(\vec{r}) \pm \psi(-\vec{r}) \right) \quad \text{sode in lihe}$$

$$P\psi_\pm = \pm \psi_\pm$$

Če E ni degenerirana je ψ sode ali liha

Zrcaljenje $\vec{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} -x \\ y \\ z \end{pmatrix}$

• Obrat časa

Klasično $m\frac{d^2\vec{r}(t)}{dt^2} = F(\vec{r},t)$

$t \to -t$

$\vec{v} \to -\vec{v}$

$\vec{a} \to \vec{a}$ če $F \neq F(t)$ je $\vec{r}(-t)$

Kvantno $V = V(\vec{r})$

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = H\psi(\vec{r},t)$$

$t \to -t$

$$i\hbar \frac{\partial \psi(\vec{r},-t)}{\partial(-t)} = H\psi(\vec{r},-t) \quad /^*$$

$H^* = H$

$$+i\hbar \frac{\partial \psi^*}{\partial(+t)} = H\psi^*$$

$$\psi(\vec{r},t) \to \psi^*(\vec{r},-t)$$

operator

$\mathcal{T}\psi = \psi^*$ $\mathcal{T} = K$ $K\psi = \psi^* K$

je operator, ki konjugira

$\psi(\vec{r},t) \to \mathcal{T}\psi(\vec{r},-t)$ minus pri t damo mi.

Primer: • $\psi = e^{i\frac{p}{\hbar}x - i\frac{E}{\hbar}t} = \psi(x,t)$

$$\psi(x,t) = \mathcal{T}\psi(x,-t) = \left(e^{-i\frac{p}{\hbar}x + i\frac{E}{\hbar}t}\right)^* = e^{i\frac{p}{\hbar}x - i\frac{E}{\hbar}t}$$

• Stacionarno stanje $\psi(\vec{r})$

$H\psi = E\psi$

$\mathcal{T}H\psi = H\mathcal{T}\psi = E\mathcal{T}\psi$ če je ψ rešitev $\Rightarrow \psi^*$ tudi

$$\Rightarrow \varphi = \frac{1}{\sqrt{2}}(\psi + \psi^*)$$

Če E ni degeneriran je $\psi = e^{i\delta}\tilde{\psi}$ $\tilde{\psi} \in \mathbb{R}$

Vrtilna količina

• $\frac{d}{dt}\langle(\vec{r}\times\vec{p})\rangle = \langle\vec{M}\rangle$, $\vec{M} = \vec{r}\times\vec{F} = \vec{r}\times(-\nabla V)$

• $U = e^{-i\varphi\,\vec{n}\cdot\vec{L}}$ $\vec{L} = \vec{r}\times\vec{p}$

Ali je hermitski ?

$[x_\alpha, p_\beta] = i\hbar\,\delta_{\alpha\beta}$ $\Rightarrow$ $\vec{L} = \vec{r}\times\vec{p} = \vec{L}^+$ je hermitski

$$\vec{L}^2 = \vec{L}\cdot\vec{L} = (\vec{r}\times\vec{p})\cdot(\vec{r}\times\vec{p}) = L_x^2 + L_y^2 + L_z^2 \qquad \vec{L} = (L_x, L_y, L_z)$$

Lastnosti

- $\boxed{[L_\alpha, L_\beta] = i\hbar\, \varepsilon_{\alpha\beta\gamma} L_\gamma}$ $\quad 1 \to 2 \to 3 \Rightarrow \varepsilon = 1$

  $[x_\alpha, x_\beta] = 0 \qquad [p_\alpha, p_\beta] = 0 \qquad 3 \to 2 \to 1 \Rightarrow \varepsilon = -1$

  $[x_\alpha, p_\beta] = i\hbar\, \delta_{\alpha\beta}$ $\qquad$ sicer $\varepsilon = 0$

$$[L_x, L_y] = [y p_z - z p_y, z p_x - x p_z] = [y p_z, z p_y] - [p_y z, z p_y] - [y p_z, x p_z] + [p_y z, x p_z]$$
$$= y p_x [p_z, z] + x p_y [z, p_z] = i\hbar (x p_y - y p_x) = i\hbar L_z$$

- $[L_\alpha, A_\beta] = i\hbar\, \varepsilon_{\alpha\beta\gamma} A_\gamma \qquad \vec{A} = \vec{r}, \vec{p}, \vec{L}, \ldots$ vektor

- z $\vec{L}$ komutirajoči operatorji:

  $[\vec{L}, A] = 0 \qquad U(\vec{\varphi}) A = A\, U(\vec{\varphi})$

  če rotacija ne spremeni A potem komutira z $\vec{L}$.

  $A = c \in \mathbb{C}$

  $A = \vec{r} \cdot \vec{r} = r^2 = |\vec{r}|^2$

  $A = p^2$

  $A = L^2 \quad \Rightarrow \quad [L_\alpha, L^2] = 0$

  $[L^2, H] = 0 \qquad H = \frac{p^2}{2m} + V(|\vec{r}|)$

- Lestvični operatorji

  $L_\pm = L_x \pm i L_y = (L_\mp)^\dagger \quad \longleftrightarrow \quad a \sim L_-$, $a^\dagger \sim L_+$

  $\boxed{[L^2, L_\pm] = 0}$

  $[L_z, L_\pm] = [L_z, L_x \pm i L_y] = [L_z, L_x] \pm i [L_z, L_y] = i\hbar L_y \pm \hbar L_x = \hbar (L_x \pm i L_y) = \pm\hbar L_\pm$

  $\boxed{[L_z, L_\pm] = \pm\hbar L_\pm}$

  $L_\pm L_\mp = (L_x \pm i L_y)(L_x \mp i L_y) = L_x^2 + L_y^2 \pm i L_y L_x \mp i L_x L_y \; (+ L_z^2 - L_z^2)$
  $= L^2 \pm i [L_y, L_x] - L_z^2 = L^2 \pm \hbar L_z - L_z^2$

  $L_\pm L_\mp = L^2 \pm \hbar L_z - L_z^2$

  $\boxed{[L_+, L_-] = 2\hbar L_z}$

Ponovitev

- $\vec{L} = \vec{r} \times \vec{p} = -\vec{p} \times \vec{r} = \vec{L}^\dagger$
- $[L_\alpha, L_\beta] = i\hbar\, \varepsilon_{\alpha\beta\gamma} L_\gamma$
- $[L_z, L_\pm] = L_z L_\pm - L_\pm L_z = \pm\hbar L_\pm$
- $L_\pm L_\mp = L^2 - L_z^2 \pm \hbar L_z$

Lastne vrednosti L_z, L^2

$L_z |m\rangle = m\hbar |m\rangle$ $\quad m \in \mathbb{R}$ $\quad \boxed{L_z = -i\hbar \frac{\partial}{\partial\varphi}}$

$-i\hbar \frac{\partial}{\partial \varphi}\psi_m(\varphi) = m\psi_m(\varphi) \Rightarrow \psi_m(\varphi) = C_m e^{im\varphi}$ ...

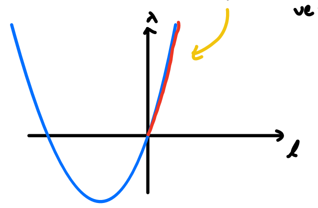
- $L_z L_\pm |m\rangle = (L_\pm L_z \pm \hbar L_\pm)|m\rangle = (m\pm1)\hbar \underbrace{L_\pm|m\rangle}_{\propto |m\pm1\rangle}$
- $[L^2, L_z]=0$ $\quad (L_x, L_y, L_z)=\vec L$

$L^2|m\rangle = \lambda|m\rangle$ $\quad \lambda\in\mathbb{R}$ ker L hermitski

$$\langle m|L^2|m\rangle = \langle m|\sum_\alpha L_\alpha^2|m\rangle = \sum_\alpha \langle L_\alpha m|L_\alpha m\rangle \geq 0$$
$$= \lambda \underbrace{\langle m|m\rangle}_{\geq 0} \Rightarrow \lambda \geq 0$$

$$L^2 L_\pm|m\rangle = L_\pm L^2|m\rangle = \lambda \underbrace{L_\pm|m\rangle}_{\text{tudi lastno stanje}}$$

Izberemo si $\lambda = \ell(\ell+1)\hbar^2$



samo te veljavni

$\lambda \leftrightarrow \ell$ bijektivno

$L^2|\ell m\rangle = \ell(\ell+1)\hbar^2|\ell m\rangle$
$L_z|\ell m\rangle = m\hbar|\ell m\rangle$

Kakšna sta ℓ, m ?

$$\langle \underbrace{L_\pm\psi_{\ell m}|L_\pm\psi_{\ell m}}_{\geq 0}\rangle = \langle\psi_{\ell m}|(L_\pm)^\dagger L_\pm\psi_{\ell m}\rangle = \langle\psi_{\ell m}|L_\mp L_\pm|\psi_{\ell m}\rangle = \langle \ell m|L^2-L_z^2 \mp \hbar L_z|\ell m\rangle =$$
$$= \langle\ell m|L^2|\ell m\rangle - \langle \ell m|L_z^2|\ell m\rangle \mp\hbar\langle\ell m|L_z|\ell m\rangle = (\underbrace{\ell(\ell+1)\hbar^2 - m(m\pm1)\hbar^2}_{\geq 0})\langle \ell m|\ell m\rangle \geq 0$$

$m\geq 0,\ \ell\geq 0$ $\quad m(m+1)\leq\ell(\ell+1) \Rightarrow m\leq\ell$
$\Downarrow$
$m\leq 0,\ \ell\geq 0$ $\quad -m\geq-\ell \Rightarrow \boxed{|m|\leq\ell}$

$$L_\pm|\ell m\rangle = \hbar\sqrt{\ell(\ell+1)-m(m\pm1)}\,|\ell, m\pm1\rangle$$
$$|\ell, m\pm1\rangle = \frac{1}{\hbar\sqrt{\ell(\ell+1)-m(m\pm1)}} L_\pm|\ell m\rangle$$

Naj bo $m=\ell$

$L_-|\ell\ell\rangle = C_{\ell,\ell-1}|\ell,\ell-1\rangle$
$L_-L_-|\ell\ell\rangle = C_{\ell,\ell-2}|\ell,\ell-2\rangle$
$\vdots$
$L_-^k|\ell\ell\rangle = C_{\ell,\ell-k}|\ell,\underbrace{\ell-k}_{-\ell}\rangle$ naj bo $\quad \ell-k=-\ell \Rightarrow 2\ell=k \Rightarrow \ell=\frac{k}{2}$
$\Rightarrow \ell = 0, \frac12, 1, \frac32, 2, \frac52, \dots$

$$\boxed{\begin{aligned} &L_z|\ell m\rangle = m\hbar\,|\ell m\rangle \\ &L^2|\ell m\rangle = \ell(\ell+1)\hbar^2|\ell m\rangle \\ &\ell = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \dots \qquad |m| \le \ell \end{aligned}}$$

V atomu so ℓ, m cela števila, brez polovičk.

Rešitve (funkcije)

Sferični harmoniki $\quad Y_\ell^m(\theta,\varphi) \qquad \langle r|\ell m\rangle = \psi_r\, Y_\ell^m$

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

$$Y_1^0 = \sqrt{\frac{3}{8\pi}}\cos\theta \qquad Y_1^1 = -\sqrt{\frac{3}{4\pi}}\sin\theta\, e^{i\varphi}$$

Obstajajo tudi realni harmoniki $\quad Y_{\ell m} \dots \cos\varphi$

Orbitale $\quad s, p, d, f$

$\qquad p_x \,,\ d_{xy} \,,\ d_{z^2}$

Zapis L z matriko

$$|\psi\rangle = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} c_{\ell m}|\ell m\rangle$$

$$L_+ = \sum_{nn'} |n\rangle\langle n|L_+|n'\rangle\langle n'| \qquad \text{splošno}$$

$$L_+ = \sum_{\substack{\ell\ell' \\ mm'}} |\ell' m'\rangle \underbrace{(L_+)_{\substack{\ell\ell' \\ mm'}}}_{\text{matrični element}} \langle \ell m|$$

$$(L_+)_{\substack{\ell\ell' \\ mm'}} = \langle \ell' m'|L_+|\ell m\rangle = \langle \ell' m'|\hbar\sqrt{\ell(\ell+1)-m(m+1)}\,|\ell, m+1\rangle\ \delta_{\ell'\ell}\ \delta_{m', m+1}$$

$$L_+|\psi\rangle \dots \hbar \begin{bmatrix} \begin{array}{c|ccc|ccccc} 0 & & 0 & & & & 0 & & \\ \hline & 0 & \sqrt{2} & 0 & & & & & \\ 0 & 0 & 0 & \sqrt{2} & & & 0 & & \\ & 0 & 0 & 0 & & & & & \\ \hline & & & & 0 & \sqrt{4} & 0 & 0 & 0 \\ & & & & 0 & 0 & \sqrt{6} & 0 & 0 \\ 0 & & 0 & & 0 & 0 & 0 & \sqrt{6} & 0 \\ & & & & 0 & 0 & 0 & 0 & \sqrt{4} \\ & & & & 0 & 0 & 0 & 0 & 0 \end{array} & \ddots \end{bmatrix} \begin{bmatrix} c_{00} \\ \hline c_{11} \\ c_{10} \\ c_{1-1} \\ \hline c_{22} \\ c_{21} \\ c_{20} \\ c_{2-1} \\ c_{2-2} \\ \vdots \end{bmatrix}$$

DN $\quad \ell = 1$

$$L_x = \frac{\hbar}{\sqrt{2}}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \qquad L_y = \frac{\hbar}{\sqrt{2}}\begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix} \qquad L_z = \frac{\hbar}{\sqrt{2}}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

Centralni potencial $V(r)$

$H = \frac{p^2}{2m} + V(r)$ invariantno na rotacije

$[H, \vec{L}] = 0$ $[H, L^2] = 0$ $\vec{r}\cdot\vec{L} = 0$ $\vec{p}\cdot\vec{L} = 0$

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + (\theta, \varphi)$$

$$H = -\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r}\right) + \frac{\vec{L}^2}{2mr^2} + V$$

$$\Psi(r,\theta,\varphi) = \psi(r)\, Y_l^m(\theta,\varphi)$$

$$H\Psi = E\Psi$$

$$\left(-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r}\right) + \underbrace{\frac{l(l+1)\hbar^2}{2mr^2} + V(r)}_{V_{eff}(r)}\right)\Psi = E\Psi$$

efektivni potencial

$\psi(r) = \frac{u(r)}{r}$ 3D (v 2D $\psi = \frac{u(r)}{\sqrt{r}}$, 1D $\psi = u(r)$)

$$\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r}\frac{u(r)}{r} = \frac{1}{r^2}\frac{\partial}{\partial r} r^2\left(\frac{u'}{r} - \frac{u}{r^2}\right) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(u'r - u\right) = \frac{1}{r^2}\left(u''r + u' - u'\right) = \frac{u''}{r} = \frac{1}{r}\frac{\partial^2 u}{\partial r^2}$$

$$\Rightarrow \left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V_{ef}(r)\right)u(r) = E\,u(r) \qquad V_{ef} = V + \frac{l(l+1)\hbar^2}{2mr^2}$$

pesti na enostavnejšo enačbo.

Lastnosti rešitev

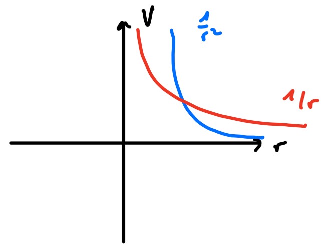
(a) $r \to 0$ omejimo se na primere, kjer velja $\lim_{r\to 0} r^2 V(r) = 0$

$V(r)$ zanemarimo

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u = \frac{l(l+1)\hbar^2}{2mr^2}u$$

zanemarili energijo

Nastavek $u = C r^\lambda$



$$-\lambda(\lambda-1) = l(l+1) \qquad \lambda_{1,2} = l+1,\ -l$$

$$u(r) = C_l r^{l+1} + D_l \frac{1}{r^l}$$

$l > 0$ $\langle\Psi,\Psi\rangle = \underbrace{\int |Y_l^m| \, d\Omega}_{1} \int_0^\infty |\psi|^2 r^2 dr < \infty$

$\supset \frac{|u|^2}{r^2}$ $\Rightarrow D_l = 0$ v limiti

$l = 0$ $u = C_0 r + D_0$

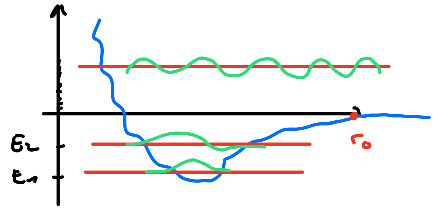
$$\int |\psi|^2 r^2 dr \xrightarrow[r\to 0]{} \frac{|D_0|^2}{r^2} r^2 = |D_0|^2$$

$\Rightarrow \psi = C_l r^l$ za $\forall l$ za $r \to 0$

(b) $r \to \infty$

• $E > 0$

$V \to 0$ dovolj hitro



$V = 0$ za $r > r_0$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u = Eu \qquad V_{ef} \to 0$$

$$u(r) = C_+ e^{ikr} + C_- e^{-ikr}$$

$$E_k = \frac{\hbar^2 k^2}{2m}$$

• $E < 0$

$$u(r) = D_+ e^{\kappa r} + D_- e^{-\kappa r} \qquad E_\kappa = -\frac{\hbar^2 \kappa^2}{2m}$$

$D_+ = 0$ zaradi normalizacije

$$u(r) = \underbrace{r^{l+1}}_{\text{majhne razdalje}} v(r) \underbrace{e^{-\kappa r}}_{\text{velike razdalje}}$$

Velja za

Coulombski potencial

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2mr^2} - \frac{e_0^2}{4\pi\varepsilon_0 r}\right)u = Eu \qquad \psi(\vec{r}) = \frac{u(r)}{r} Y_l^m(\theta,\varphi)$$

$E = ?$

$$\rho = \kappa r, \quad |E| = \frac{\kappa^2\hbar^2}{2m} \qquad \rho_0 = \frac{m e_0^2}{2\pi\varepsilon_0 \hbar \kappa}$$

$$/\cdot\frac{1}{\kappa^2}\frac{2m}{\hbar^2} \Rightarrow \left(-\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2} + \underbrace{\frac{\rho_0}{\rho}}_{V} \underbrace{-1}_{E}\right)u = 0$$

$$u(r(\rho)) \to u(\rho)$$

Že vemo $u(\rho) = \rho^{l+1} v(\rho) e^{-\rho}$ $\quad \frac{du}{dr} = \dots \Rightarrow \frac{d^2u}{dr^2} = \dots$

Vstavimo v enačbo in preuredimo da dobimo

$$\rho v'' + 2(l+1-\rho)v' + (\rho_0 - 2(l+1))v = 0$$

Rešimo z razvojem v vrsto.

$$v(\rho) = \sum_{k=0}^{\infty} c_k \rho^k \qquad \text{nastavek}$$

$$v'(\rho) = \sum_{k=0}^{\infty} c_k k \rho^{k-1} = \sum_{k=0}^{\infty} (k+1) c_{k+1} \rho^k$$

$$v''(\rho) = \sum_{k=0}^{\infty} k(k-1) c_k \rho^{k-2} = \sum_{k=0}^{\infty} k(k+1) c_{k+1} \rho^{k-1}$$

$$\sum_{k=0}^{\infty} k(k+1)\, c_{k+1}\, \rho^k + 2(\ell+1-\rho)(k+1)\, c_{k+1}\, \rho^k + (\rho_0 - 2(\ell+1))\, c_k\, \rho^k = 0$$

$$\sum_{k=0}^{\infty} \rho^k \left[\left(k(k+1) + 2(\ell+1)(k+1)\right) c_{k+1} + \left(-2k + \rho_0 - 2(\ell+1)\right) c_k \right] = 0$$

$$c_{k+1} = c_k \, \frac{2(k+\ell+1) - \rho_0}{(k+1)\,(k+2(\ell+1))}$$

Limita $k \gg 1$

$$c_{k+1} \approx c_k \frac{2k}{k^2} = c_k \frac{2}{k}$$

$$e^{2x} = \sum_{k=0}^{\infty} \frac{2^k x^k}{k!} \Rightarrow \frac{2^{k+1}}{(k+1)!} \frac{k!}{2^k} = \frac{2}{k+1} \to \frac{2}{k}$$

Torej $v(\rho) \to e^{2\rho} \quad (\rho \to \infty,\ k \to \infty)$

$$u(\rho) = \rho^{\ell+1} e^{2\rho} e^{-\rho} = \rho^{\ell+1} e^{\rho}$$ Ni normalizabilno

Tega ne želimo, zato $\exists\, k_{max}: \underbrace{2(k_{max}+\ell+1) - \rho_0}_{\text{ustavi rekurzivno zvezo}} = 0 \Rightarrow c_{k_{max}+1} = 0$

Omejili smo vrsto $\sum_{k=0}^{k_{max}} c_k \rho^k = v(\rho)$ polinom reda k_{max} (in ne eksponenta)

$k = 0, 1, 2, \dots, k_{max}$; $n = k_{max} + \ell + 1 \geq 1$ $\quad \rho_0 = 2n = 2, 4, 6, \dots$

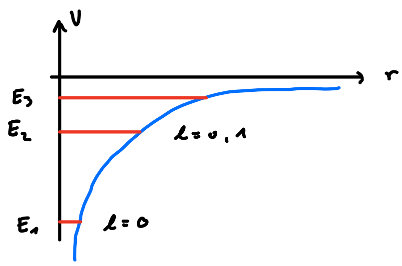
$$E = -\frac{\kappa^2 \hbar^2}{2m} = -\frac{m e_0^2}{8\pi^2 \varepsilon_0^2 \hbar^2 \rho_0^2}$$

$$E_n = -\frac{m}{2\hbar^2}\left(\frac{e_0^2}{4\pi\varepsilon_0}\right)^2 \frac{1}{n^2} = -\frac{|E_1|}{n^2}$$ $\quad |E_1| = 1\,Ry = 13{,}6\,eV$ Rydberg

Degeneracija

$$E_n = -\frac{1 Ry}{n^2} \qquad n = k+\ell+1 \qquad k = 0, 1, \dots \qquad \ell = 0, 1, \dots$$

n	ℓ	k
1	0	0
2	1	0
	0	1
3	2	0
	1	1
	0	2
	$\vdots$	

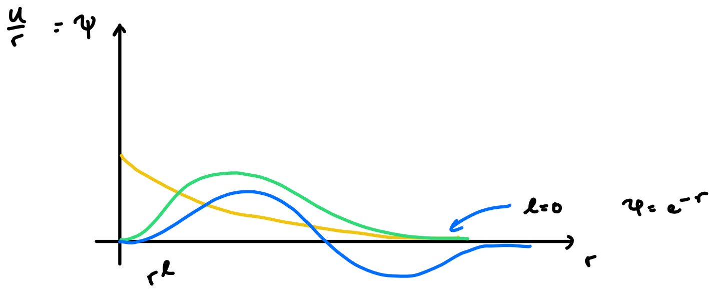


$\ell = 0, 1, \dots, n-1$

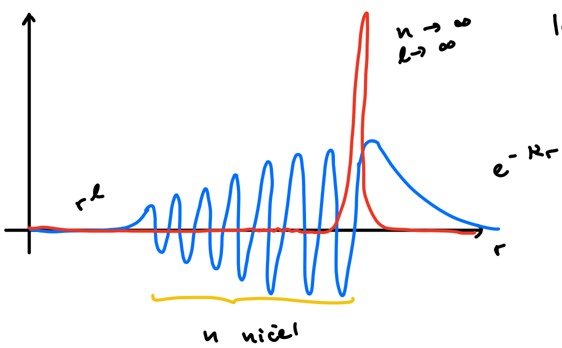
$m = \underbrace{-\ell, -\ell+1, \dots, \ell}_{2\ell+1}$

Število m-jev pri istem n $\quad \sum_{\ell=0}^{n-1} (2\ell+1) = n^2 \quad$ Degeneracija je n^2.

Klasična limita



Klas. limita $n >> 1$, $l >> 1$



lokaliziran nadij → e^- se giblje na konst. orbiti.

Kvantni Laplace – Runge – Lenzov vektor

$$\vec{A} = \frac{1}{2}\Big(\vec{p} \times \vec{L} + \underbrace{(\vec{p} \times \vec{L})^\dagger}_{-\vec{L} \times \vec{p}}\Big) - \frac{m e_0^2}{4\pi\varepsilon_0} \frac{\vec{r}}{r}$$

$$[\vec{L}, H] = 0$$
$$[L^2, H] = 0$$
$$[\vec{A}, H] = 0$$
$$\vec{A} \cdot \vec{L} = \vec{L}\,\vec{A} = 0$$
$$[L_\alpha, L_\beta] = i\hbar\, \varepsilon_{\alpha\beta\gamma} L_\gamma$$
$$[L_\alpha, A_\beta] = i\hbar\, \varepsilon_{\alpha\beta\gamma} A_\gamma$$
$$[A_\alpha, A_\beta] = i\hbar\, \varepsilon_{\alpha\beta\gamma} A_\gamma \quad \dots \quad \rightarrow \quad E_n$$

Nabit delec v magnetnem polju

Klasično $\quad m\vec{a} = e\vec{E} + e\vec{v} \times \vec{B}$

Kvantno $\quad H = \dfrac{(\vec{p} - e\vec{A})^2}{2m} + e\varphi$

$$\vec{B} = \nabla \times \vec{A}$$
$$\vec{E} = -\nabla\varphi - \frac{\partial}{\partial t}\vec{A}$$

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{1}{2m}\left(-i\hbar\nabla - e\vec{A}\right)^2 \psi + e\varphi\,\psi$$

$$(\nabla \cdot \vec{A})\,\psi + (\vec{A} \cdot \nabla)\,\psi = \nabla A \psi + \vec{A}\,\nabla\psi = 2\vec{A}\,\nabla\psi + \psi\,\nabla\vec{A}$$

$$\Rightarrow \quad i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + \underbrace{i\frac{\hbar e}{m}\vec{A}\,\nabla\psi}_{\text{Zeeman}} + \left(i\frac{\hbar e}{m}(\nabla\vec{A}) + \frac{e^2}{2m}A^2 + e\varphi\right)\psi$$

EMP $\quad \nabla\vec{A} = 0 \quad$ Coulombove umeritve

• Zeemanova sklopitev

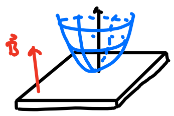
$\nabla \vec{A} = 0 \quad , \quad \vec{A} = -\frac{1}{2}(\vec{r}\times\vec{B}) \qquad \vec{B} = \text{konst.} = (0, 0, B)$

$$i\frac{\hbar e}{m}\vec{A}\,\nabla\psi = -i\frac{\hbar e}{2m}\underbrace{(\vec{r}\times\vec{B})\,\nabla\psi}_{\text{mešan produkt}} = i\frac{\hbar e}{2m}(\vec{r}\times\nabla)\vec{B}\,\psi = -\frac{e}{2m}(\vec{r}\times\vec{p})\vec{B}\,\psi =$$

$$= -\frac{e}{2m}\vec{B}\,\vec{L}\,\psi$$

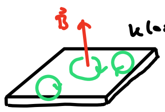
$H_{zeeman} = -\vec{\mu}\,\vec{B} \qquad \vec{\mu} = \frac{e}{2m}\vec{L}$

• $H_2 = \frac{e^2}{2m}\vec{A}\cdot\vec{A} = \frac{e^2B^2}{8m}(x^2+y^2) \qquad \vec{A} = \frac{B}{2}(-y, x, 0)$



$\frac{H_2}{H_Z} \sim 10^{-6} \Rightarrow H_2$ zanemarljiv (dokler nismo v kon. polju)

Homogeno magnetno polje: Landauovi nivoji



$\vec{B} = B\hat{e}_z \qquad \vec{A} = -\frac{1}{2}(\vec{r}\times\vec{B}) = \frac{B}{2}(-y, x, 0)$

ali $\vec{A} = B(y, 0, 0)$ ← Landauova umeritev

ali $\vec{A} = B(0, x, 0)$

$\Rightarrow \nabla\times\vec{A} = \vec{B}$

Landauova umeritev $\vec{A} = B(y, 0, 0)$
↓

$$\frac{1}{2m}\Big(\underbrace{\left(-i\hbar\frac{d}{dx} + eBy\right)^2}_{f(p)} - \hbar^2\frac{\partial^2}{\partial y^2} - \hbar^2\frac{\partial^2}{\partial z^2}\Big)\psi + e\varphi\psi = E\psi$$

Nastavek $\psi(\vec{r}) = e^{i\left(\frac{p_x}{\hbar}x + \frac{p_z}{\hbar}z\right)}\chi(y) \qquad$ Naj bo $\varphi = \varphi(y)$
$= 0$

Splošno $\hat{A}$, $f(\hat{A})\psi = f(a)\psi_a$
ψ lastna funkcija $\hat{A} \qquad \hat{A}\psi_a = a\psi_a$

$$f\left(-i\hbar\frac{\partial}{\partial x}\right)e^{i\frac{p_x}{\hbar}x} = f(p_x)\,e^{i\frac{p_x}{\hbar}x}$$

$$\frac{1}{2m}\left((p_x + eBy)^2 - \hbar^2\frac{\partial^2}{\partial y^2}\right)\chi + V(y)\chi = E\chi$$

$$V(y) = e\varphi(y) + \frac{p_z^2}{2m}$$

Naj bo $V = 0$:

$\omega = \frac{eB}{m}$ ciklotronska frekvenca

$\xi = \sqrt{\frac{\hbar}{eB}}$ magnetna dolžina

$p_x = \hbar k \qquad y_k = -\xi^2 k = -\frac{\hbar}{eB}k$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dy^2} + \frac{1}{2}m\omega^2(y-y_k)^2\right)\chi = E_n\chi \qquad E_n = \hbar\omega(n + 1/2)$$

↑ premaknjen harmonski oscilator

$$\psi_{n,k}(x,y) = \frac{1}{\sqrt{2\pi}}e^{ikx}\varphi_n(y-y_k)$$

→ n-ta rešitev za harmonski oscilator

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

$\Rightarrow$ degeneracija

Razvoj po ravnih valovih

$$\psi(x,0) = \int_{-\infty}^{\infty} \tilde{\psi}(k)\,\frac{e^{ikx}}{\sqrt{2\pi}}\,dk$$

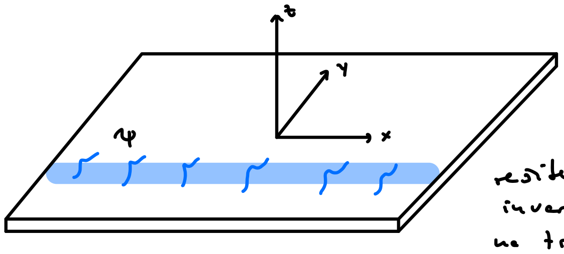
$$\psi(x,t) = \int_{-\infty}^{\infty} \tilde{\psi}(k)\,\frac{e^{ikx - i\frac{E_n}{\hbar}t}}{\sqrt{2\pi}}\,dk$$

$$= e^{-i\frac{E_n}{\hbar}t}\int_{-\infty}^{\infty} \tilde{\psi}(k)\,\frac{e^{ikx}}{\sqrt{2\pi}}\,dk$$

$$= e^{-i\frac{E_n}{\hbar}t}\,\psi(x,0)$$

$$|\psi(x,t)|^2 = |\psi(x,0)|^2$$

paket se ne premika



rešitev invariantna na translacijo v x smeri

Lokalne umeritvene transformacije

$\vec{B} = \nabla \times \vec{A}$

$\vec{E} = -\nabla\varphi$

Lahko upeljemo nov $\vec{A}$

$\vec{A}' = \vec{A} + \nabla\Lambda \qquad B' = B$

$\varphi' = \varphi - \frac{\partial}{\partial t}\Lambda \qquad E' = E$

Rešitev odvisna od izbire $\vec{A}$ (čudno)

Kaj se zgodi s ψ. ($\psi \to \psi' = ?$)

Vpeljimo ψ':

$\psi'(\vec{r},t) = e^{i\sigma(\vec{r},t)}\,\psi(\vec{r},t) \qquad \sigma \in \mathbb{R}$

damo v Sch.

$$i\hbar\frac{\partial}{\partial t}\psi' = \frac{1}{2m}\big(-i\hbar\nabla \underbrace{-e\vec{A}'}_{f}\big)^2\psi' + e\varphi'\psi'$$

Želimo izraziti φ' in $\vec{A}'$ s φ in $\vec{A}$.

$$\left(i\frac{\partial}{\partial x} + f\right)e^{i\sigma}\psi = -\left(\frac{\partial\sigma}{\partial x}\right)e^{i\sigma}\psi + e^{i\sigma}i\frac{\partial\psi}{\partial x} + f e^{i\sigma}\psi$$

$$= e^{i\sigma}\left(i\frac{\partial}{\partial x} + \left(f - \frac{\partial\sigma}{\partial x}\right)\right)\psi$$

$$\left(i\frac{\partial}{\partial x} + f\right)^2 e^{i\sigma}\psi = \left(i\frac{\partial}{\partial x} + f\right)e^{i\sigma}\left(i\frac{\partial}{\partial x} + \left(f - \frac{\partial\sigma}{\partial x}\right)\right)\psi = e^{i\sigma}\left(i\frac{\partial}{\partial x} + \left(f - \frac{\partial\sigma}{\partial x}\right)\right)^2\psi \quad /: e^{i\sigma}$$

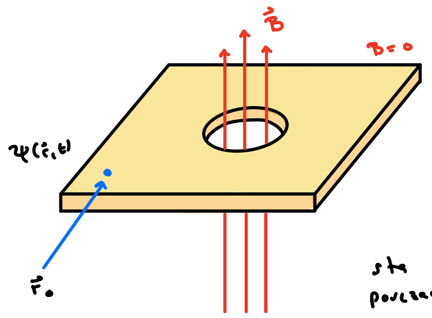
$$i\hbar\frac{\partial}{\partial t}\psi = \frac{1}{2m}\sum_{\alpha=x}^{z}\left(-i\hbar\frac{\partial}{\partial x_\alpha} - eA_\alpha + \hbar\frac{\partial\sigma}{\partial x_\alpha}\right)^2\psi + \left(e\varphi' + \hbar\frac{\partial\sigma}{\partial t}\right)\psi$$

$$i\hbar\frac{\partial}{\partial t}\psi = \left(\frac{(\vec{p}-e\vec{A})^2}{2m} + e\phi\right)\psi \qquad \Lambda = \frac{\hbar}{e}\sigma$$

$\psi'(\vec{r},t) = e^{i\frac{e}{\hbar}\Lambda(\vec{r},t)}\,\psi(\vec{r},t)$ Rešitev Schrod. en. pri drugem $\vec{A}' = \vec{A} + \nabla\Lambda$

$\rho' = |\psi'|^2 = |\psi|^2 = \rho$ $\qquad \psi$ se spremeni, ρ pa se ne

Aharonov – Bohmov pojav



$$\vec B = \nabla \times \vec A = 0$$
$$\Rightarrow \quad \vec A = \nabla \Lambda$$
$$\Lambda(\vec r,t) = \Lambda(\vec r_0,t) - \int_{\vec r_0}^{\vec r} \vec A(\vec r')\,d\vec r'$$
po neki poti

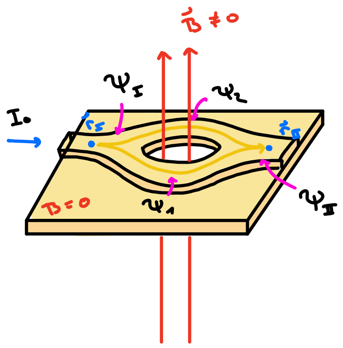
sta povezana
$$\psi_A : \quad i\hbar \frac{\partial \psi_A}{\partial t} = \frac{(\vec p - e\vec A)^2}{2m}\psi_A + V\psi_A$$
$$\psi_0 : \quad i\hbar \frac{\partial \psi_0}{\partial t} = \frac{p^2}{2m}\psi_0 + V\psi_0$$

$\vec B = 0$

$$\vec A' = \vec A + \underbrace{\nabla(-\Lambda)}_{-\vec A} = 0$$
$$\psi_A(\vec r,t) = e^{-i\frac{e}{\hbar}\Lambda(\vec r,t)}\,\psi_0$$

Vstavimo Λ

$$\psi_A(\vec r,t) = e^{i\frac{e}{\hbar}\int_{\vec r_0}^{\vec r}\vec A(\vec r')\,d\vec r'}\,\psi_0(\vec r,t)$$

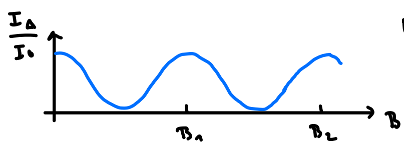


$$\psi_{II} = \psi_1 + \psi_2$$
$$\psi_{IIA} = e^{i\delta_1}\psi_1 + e^{i\delta_2}\psi_2$$
$$= e^{i\delta_2}\left(e^{i\delta_1 - i\delta_2}\psi_1 + \psi_2\right)$$
$$= e^{i\delta_2}\psi_1\left(1 + e^{i(\delta_1-\delta_2)}\right)$$

$$\delta_{1,2} = \frac{e}{\hbar}\int_{r_I}^{r_{II}} \vec A(\vec r)\,d\vec r \quad \text{pot 1, pot 2}$$
$$\psi_1 \simeq \psi_2$$

$$\delta_1 - \delta_2 = \frac{e}{\hbar}\oint_{pot} \vec A(\vec r)\,d\vec r = \frac{e}{\hbar}\Big(\int_{I,\,pot1}^{II} - \int_{I,\,pot2}^{II}\Big) =$$
$$= \frac{e}{\hbar}\iint_S (\nabla\times\vec A)\,d\vec S = \frac{e}{\hbar}\iint_S \vec B\,d\vec S = \frac{e}{\hbar}\Phi_m$$

ko $B \neq 0$
$$\frac{I_A}{I_0} = \frac{|\psi_{IIA}|^2}{|\psi_{II0}|^2} = \frac{1}{4}\left|1 + e^{i\frac{e}{\hbar}\Phi_m}\right|^2 = \cos^2\frac{e}{2\hbar}\Phi_m$$
ko je $B=0$



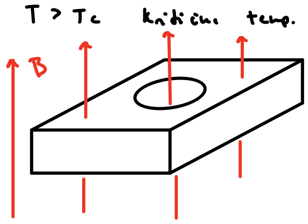
$$\boxed{I_A = I_0 \cos^2\frac{e}{2\hbar}\Phi_m}$$

Minimumi in maksimumi $\quad \frac{e}{2\hbar}\Phi_m = n\pi \qquad \Phi_m = \frac{n\pi 2\hbar}{e} = n\frac{h}{e}$

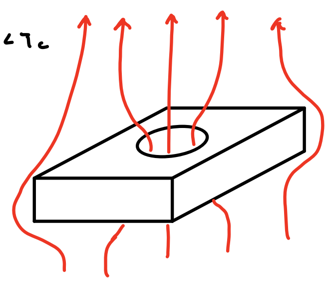
Lahko uporabimo za merjenje $\vec B$. (Hall sensor)

Levitacija

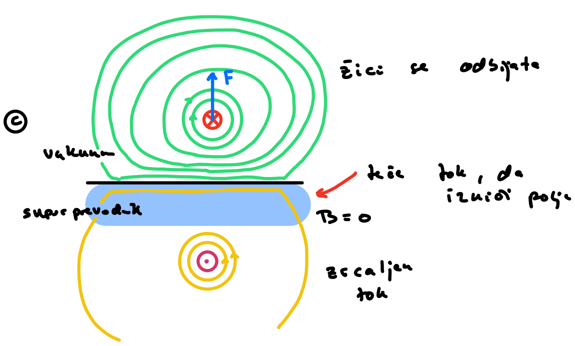
a) $T > T_c$ kritična temp.



b) $T < T_c$



c)



Spin

$\vec{r} \times \vec{p} = \vec{L} \quad : \quad l = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots \qquad [L_\alpha, L_\beta] = i\hbar\, \varepsilon_{\alpha\beta\gamma} L_\gamma$

Za H-atom rabimo le celoštevilske l. Kaj pa če uporabimo polovična števila.

$$[S_\alpha, S_\beta] = i\hbar\, \varepsilon_{\alpha\beta\gamma} S_\gamma$$

$$s = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$$

$$S_\pm = S_x \pm i S_y$$

zanima nas $s = \frac{1}{2}$ ker je tu

$$|s\ m_s\rangle = |s\ m\rangle = |\tfrac{1}{2}\ m\rangle = |m\rangle = \begin{matrix}|1\rangle \\ |0\rangle\end{matrix}$$

spinor $\begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}, \begin{pmatrix}c_1\\c_2\end{pmatrix}$

$$S_\pm |s\,m\rangle = \hbar\sqrt{s(s+1) - m(m\pm1)}\ |s, m\pm1\rangle$$
$$S_z |s\,m\rangle = m\hbar\, |s\,m\rangle$$
$$S^2 |s\,m\rangle = s(s+1)\hbar^2\, |s\,m\rangle$$

Od tu naprej $s = 1/2$ $\qquad |\uparrow\rangle = |\tfrac{1}{2}\rangle \quad |\downarrow\rangle = |-\tfrac{1}{2}\rangle \qquad \vec{S} = (S_x, S_y, S_z)$

$S_+ |\downarrow\rangle = \hbar |\uparrow\rangle$ $\qquad$ Spin flip (obrat spina)

$S_- |\uparrow\rangle = \hbar |\downarrow\rangle$

$$\langle\uparrow| S_+ |\uparrow\rangle = \hbar \langle\uparrow|\downarrow\rangle = 0 = \langle\downarrow| S_+ |\downarrow\rangle$$

$\langle\downarrow| \underbrace{S_+|\uparrow\rangle}_{0} = 0 \qquad \langle\uparrow| S_+ |\downarrow\rangle = \hbar \qquad$ V bazi $|\uparrow\rangle, |\downarrow\rangle$

$$S_+ = \hbar\begin{bmatrix}0 & 1\\0 & 0\end{bmatrix} \qquad S_- = S_+^\dagger = \hbar\begin{bmatrix}0 & 0\\1 & 0\end{bmatrix} \qquad \begin{array}{c|cc} & |\uparrow\rangle & |\downarrow\rangle \\ \hline |\uparrow\rangle & & \\ |\downarrow\rangle & & \end{array}$$

Spinske operatorje na zapišemo eksplicitno kvečjemu z matričnimi elementi.

$$S_x = \frac{1}{2}(S_+ + S_-) = \frac{\hbar}{2}\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix} = S_x^\dagger$$
$$S_y = \frac{1}{2i}(S_+ - S_-) = \frac{\hbar}{2}\begin{bmatrix}0 & -i\\i & 0\end{bmatrix} = S_y^\dagger$$
$$S_z = \frac{\hbar}{2}\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$$

$$S_x^2 = \frac{\hbar^2}{4}\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix} = \frac{\hbar^2}{4}\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix} = S_y^2 = S_z^2$$

$$[S_\alpha, S_\beta^2] = 0$$

$$S^2 = \sum_\beta S_\beta^2$$

$$[S_\alpha, S^2] = 0$$

$$S_+ = \frac{\hbar}{2}\left[\begin{array}{cc|cccc|c} 0 & 1 & & & & & \\ 0 & 0 & & & 0 & & 0 \\ \hline & & 0 & \sqrt{3} & 0 & 0 & \\ & 0 & 0 & 0 & 2 & 0 & 0 \\ & & 0 & 0 & 0 & \sqrt{3} & \\ & & 0 & 0 & 0 & 0 & \\ \hline & 0 & & & 0 & & \ddots \end{array}\right] \qquad \text{za } s \text{ ki ni samo } \tfrac{1}{2}.$$

$$\begin{array}{ccc} \tfrac{1}{2} & \tfrac{3}{2} & \dots \end{array}$$

Paulijeve matrike

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma} = \frac{\hbar}{2}(\sigma_x, \sigma_y, \sigma_z)$$

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$H = E_0 I + \sum_\alpha E_\alpha \sigma_\alpha = H^\dagger \qquad E_0, E_\alpha \in \mathbb{R}$$

Lastnosti

- $\det \sigma_\alpha = -1$
- $\operatorname{tr} \sigma_\alpha = 0$
- $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I$
- $\sigma_x \sigma_y \sigma_z = iI$
- $\sigma_x \sigma_y = \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix} = i\sigma_z = -\sigma_y \sigma_x$
- $\sigma_\alpha \sigma_\beta = \delta_{\alpha\beta} I + i\varepsilon_{\alpha\beta\gamma}\sigma_\gamma$
- $[\sigma_\alpha, \sigma_\beta] = 2i\varepsilon_{\alpha\beta\gamma}\sigma_\gamma$
- $\{\sigma_\alpha, \sigma_\beta\} = \sigma_\alpha\sigma_\beta + \sigma_\beta\sigma_\alpha = 2\delta_{\alpha\beta} I$
- $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, $\vec{a} = (a_x, a_y, a_z)$

  $\vec{a}\vec{\sigma} = \sum_\alpha a_\alpha \sigma_\alpha$

  $(\vec{a}\vec{\sigma})(\vec{b}\vec{\sigma}) = \sum_{\alpha,\beta} a_\alpha \sigma_\alpha b_\beta \sigma_\beta = \sum_{\alpha\beta} a_\alpha b_\beta (\delta_{\alpha\beta} I + i\varepsilon_{\alpha\beta\gamma}\sigma_\gamma) = \vec{a}\cdot\vec{b}\, I + i(\vec{a}\times\vec{b})\vec{\sigma}$
- $\vec{a} = \vec{b} = \vec{n}$ $\quad |\vec{n}| = 1$

  $(\vec{n}\vec{\sigma})(\vec{n}\vec{\sigma}) = I$

Kvaternioni

$$q = a_0 + a_1 i + a_2 j + a_3 k \qquad \in \mathbb{H}$$

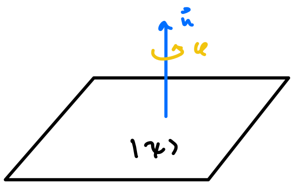
$a_i \in \mathbb{R}$

- $-1 = i^2 = j^2 = k^2 = ijk$
- $ij = -k = -ji$ ciklično

Zveza z matrikami

$$i \to \frac{1}{i}\sigma_x \qquad j \to \frac{1}{i}\sigma_y \qquad k \to \frac{1}{i}\sigma_z \qquad 1 \to I$$

Rotacija spinorjev



$$U(\varphi, \vec{n}) = e^{-i\varphi \frac{\vec{n}\cdot\vec{L}}{\hbar}}$$ zavrti ψ

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma} = \frac{\hbar}{2}(\sigma_x, \sigma_y, \sigma_z)$$

$2s+1 = 2$

$\chi(\vec{r})$ ne obstaja

$$|\chi\rangle = a|\tfrac{1}{2}\rangle + b|-\tfrac{1}{2}\rangle$$

spinor

$|m\rangle = |\pm\tfrac{1}{2}\rangle = |s\,m\rangle$, $|\uparrow\rangle\ |\downarrow\rangle$

$$\chi = \begin{pmatrix} a \\ b \end{pmatrix} = a\begin{pmatrix} 1 \\ 0 \end{pmatrix} + b\begin{pmatrix} 0 \\ 1 \end{pmatrix} = a\chi_\uparrow + b\chi_\downarrow$$

Kako zarotirati $|\chi\rangle$

$$U(\varphi,\vec n) = e^{-i\varphi \frac{\vec n\cdot\vec S}{\hbar}}$$

$$|\tilde\chi\rangle = U|\chi\rangle$$

$$e^{-i\varphi\frac{\vec n\cdot \vec S}{\hbar}} = e^{-i\varphi\frac{\vec n\cdot\vec\sigma}{2}} = \sum_{k=0}^{\infty} \frac{1}{k!}\left(-i\frac{\varphi}{2}\vec n\cdot\vec\sigma\right)^k = 1 - i\frac{\varphi}{2}\vec n\cdot\vec\sigma + \frac{1}{2}\left(-i\frac{\varphi}{2}\vec n\cdot\vec\sigma\right)^2 + \mathcal{O}((\vec n\cdot\vec\sigma)^3) = \dots$$

$$(\vec a\cdot\vec\sigma)(\vec b\cdot\vec\sigma) = \vec a\cdot\vec b + i(\vec a\times\vec b)\vec\sigma$$

$$(\vec n\cdot\vec\sigma)^2 = I$$

$$(\vec n\cdot\vec\sigma)^3 = \vec n\cdot\vec\sigma$$

$$(\vec n\cdot\vec\sigma)^k = \begin{cases} I & k \text{ sod}\\ \vec n\cdot\vec\sigma & k\text{ lih}\end{cases}$$

$$\dots = \left(1 - \frac{1}{2!}\left(\frac{\varphi}{2}\right)^2 + \frac{1}{4!}\left(\frac\varphi2\right)^4 - \dots\right)I + (-i)\left(\frac\varphi2 - \frac{1}{3!}\left(\frac\varphi2\right)^3 + \frac{1}{5!}\left(\frac\varphi2\right)^5 - \dots\right)\vec n\cdot\vec\sigma$$

$$\boxed{U(\varphi,\vec n) = \cos\frac\varphi2\, I - i\sin\frac\varphi2\, \vec n\cdot\vec\sigma}$$

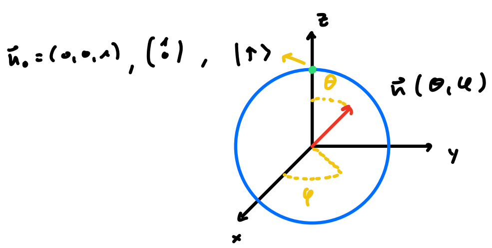
Primer: $\varphi=2\pi$

$$U(2\pi,\vec n) = \cos\pi\, I = -I$$

$$U(2\pi,\vec n)|\chi\rangle = -|\chi\rangle$$

$\chi(t)\to-\chi(t)$ ni zvezna, zato $\chi(t)$ ne obstaja

Blochova sfera



qubit = kvantni bit

$|\chi\rangle = U(\varphi,\hat e_z)U(\theta,\hat e_y)|\uparrow\rangle =$ ker σ_z in σ_y ne komutirata jih ne moremo dati na en eksponent

$= e^{-i\frac\varphi2\sigma_z}\, e^{-i\frac\theta2\sigma_y}|\uparrow\rangle$

$\chi = e^{-i\frac\varphi2\sigma_z}\left(\cos\frac\theta2\, I - i\sin\frac\theta2 \begin{pmatrix}0&-i\\i&0\end{pmatrix}\right)\binom{1}{0} =$

$= e^{-i\frac\varphi2\sigma_z}\begin{bmatrix}\cos\frac\theta2 & -\sin\frac\theta2\\ \sin\frac\theta2&\cos\frac\theta2\end{bmatrix}\binom{1}{0}$

$= e^{-i\frac\varphi2\sigma_z}\begin{pmatrix}\cos\theta/2\\ \sin\theta/2\end{pmatrix} = e^{-i\frac\varphi2\sigma_z}\left(\cos\frac\theta2\binom{1}{0} + \sin\frac\theta2\binom{0}{1}\right) =$

$= e^{-i\frac\varphi2}\cos\frac\theta2\binom{1}{0} + e^{i\frac\varphi2}\sin\frac\theta2\binom{0}{1}$

$= e^{-i\frac\varphi2}\left(\cos\frac\theta2\binom{1}{0} + e^{i\varphi}\sin\frac\theta2\binom{0}{1}\right)$

↳ val. funk. določena do faze natančno

$f(\hat A)$

$\hat A|a\rangle = a|a\rangle$

$f(\hat A)|a\rangle = f(a)|a\rangle$

$\sigma_z\binom{1}{0} = \binom{1}{0}$

$\sigma_z\binom{0}{1} = -\binom{0}{1}$

$$\boxed{|\chi_\uparrow\rangle = \underbrace{\cos\frac\theta2}_{a}|\uparrow\rangle + \underbrace{e^{i\varphi}\sin\frac\theta2}_{b}|\downarrow\rangle}$$

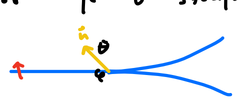
$\chi_\uparrow(\theta,\varphi)$ lahko bi izpeljali tudi $|\chi_\downarrow\rangle$

$$\chi = \begin{pmatrix}\cos\theta/2\\ e^{i\varphi}\sin\theta/2\end{pmatrix}$$

$|a|^2+|b|^2=1$

Primer: kvantni sistem je v stanju $|\chi_0\rangle = |\uparrow\rangle$. Izmerimo smer spina glede na $\vec n$.

$\vec n(\varphi,\theta)$



Zanima nas verjetnost da bo izid meritve $(\vec n\cdot\vec S) = +\frac\hbar2$

$\langle \hat A\rangle = \langle\psi|\hat A|\psi\rangle$

$|\psi\rangle = \sum c_n |\phi_n\rangle$

$\hat A|\phi_n\rangle = a_n|\phi_n\rangle$

Pri meritvi $\hat A$ bo izmerek eno od lastnih vrednosti a_n; $P_n = |c_n|^2$,

$|\psi\rangle \xrightarrow{\text{kolaps}} |\phi_n\rangle$

- $\vec n\cdot\vec s\,|\chi(\theta,\varphi)\rangle = \pm\frac{\hbar}{2}|\chi(\theta,\varphi)\rangle$

$|\chi_0\rangle = c_\uparrow|\chi_\uparrow\rangle + c_\downarrow|\chi_\downarrow\rangle \quad /\cdot\langle\chi_\uparrow|$

$\langle\chi_\uparrow|\chi_0\rangle = c_\uparrow$

$P_\uparrow(\theta,\varphi) = |\langle\chi_\uparrow|\chi_0\rangle|^2 = \cos^2\frac{\theta}{2} = 1-P_\downarrow$

- $\langle\vec\sigma\rangle = \langle\chi_\uparrow|\vec\sigma|\chi_\uparrow\rangle = (\langle\chi_\uparrow|\sigma_x|\chi_\uparrow\rangle, \langle\chi_\uparrow|\sigma_y|\chi_\uparrow\rangle, \langle\chi_\uparrow|\sigma_z|\chi_\uparrow\rangle) = \vec n$

Anomalni Zeemanov pojav

$H = -\frac{e}{2m}\vec B\cdot\vec L$ delec v magnetnem polju

Anomalni Zeemanov pojav $H = -g\frac{e}{2m}\vec B\cdot\vec S$ $\quad g = 2{,}002\ldots$ vakuum

$H = -\frac{e}{m}\vec B\cdot\vec S$

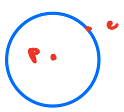
Paulijev formalizem

$\Psi(\vec r,t) = \begin{pmatrix}\psi_\uparrow(\vec r,t)\\ \psi_\downarrow(\vec r,t)\end{pmatrix} \qquad \underset{\downarrow}{\rho_\uparrow} = |\underset{\downarrow}{\psi_\uparrow}|^2 \qquad \rho = \rho_\uparrow + \rho_\downarrow \qquad \int\rho\, d^3r = 1$

$H = \left(\frac{p^2}{2m} + V - \frac{e}{2m}\vec B\cdot\vec L\right) \underset{\begin{pmatrix}1&0\\0&1\end{pmatrix}}{I} + \left(-g\frac{e}{2m}\vec B\cdot\vec S\right) + \underbrace{W(r)\,\vec L\cdot\vec S}_{\text{sklopitev spin-tir}} + \underbrace{d(\vec\sigma\times\vec p)\,\vec n}_{\text{Rashba sklopitev}} + \ldots$

Seštevanje vrtilnih količin

Vodik, osnovno stanje $|l\,m\rangle = |00\rangle \qquad \langle\vec r|00\rangle = \psi_{00}(r)$



e: $|\Psi\rangle = |00\rangle\,\underset{\text{spin elektrona}}{|\chi_e\rangle} \qquad \Psi = \psi_{00}(r)\underset{\text{ni vrtilne količine}}{\begin{pmatrix}a\\b\end{pmatrix}} \qquad |\chi\rangle_e$

p: $|\chi_p\rangle = \begin{pmatrix}c\\d\end{pmatrix} \qquad \Psi_p(\vec r) = \psi_p(\vec r)\begin{pmatrix}c\\d\end{pmatrix} \qquad |\Psi\rangle_p$

p+e: e: $|\uparrow\rangle_e, |\downarrow\rangle_e$ p: $|\uparrow\rangle_p, |\downarrow\rangle_p$

krajevni del nas ne zanima

baza
$|\uparrow\rangle_e|\uparrow\rangle_p$
$|\downarrow\rangle_e|\uparrow\rangle_p$
$|\uparrow\rangle_e|\downarrow\rangle_p$
$|\downarrow\rangle_e|\downarrow\rangle_p$

tenzorski produkt

$|\uparrow\rangle_e\otimes|\uparrow\rangle_p = |\uparrow\rangle\otimes|\uparrow\rangle$

dogovorimo, da je prvo od e, drugo od p.

Sklopno stanje $|\chi\rangle \otimes |\psi\rangle$ $\qquad \vec{S} = \frac{\hbar}{2}\vec{\sigma} = \frac{\hbar}{2}(\sigma_x, \sigma_y, \sigma_z)$

delovanje operatorja $S_{ez}|\uparrow\rangle_e = \frac{\hbar}{2}|\uparrow\rangle_e$ $\qquad S_{pz}|\downarrow\rangle_p = -\frac{\hbar}{2}|\downarrow\rangle_p$

Vsota operatorjev $\vec{S}_e, \vec{S}_p$ $\qquad \vec{S}_{p,e} = \frac{\hbar}{2}\vec{\sigma}_{p,e}$

$$\boxed{\vec{S} = \vec{S}_e \otimes I_p + I_e \otimes \vec{S}_p}$$

identiteta v bazi protona

Naj so $\vec{S}_e = \vec{S}_1$, $\vec{S}_p = \vec{S}_2$

Baza za 2 delca

- $|s_1 m_1\rangle \otimes |s_2 m_2\rangle = |\Psi\rangle$

$\vec{S}_1|\Psi\rangle = |\tilde{\Psi}\rangle$

$\vec{S}_1 \to \vec{S}_1 \otimes I_2$

$\phi(x,y) = \varphi_1(x)\varphi_2(y)$

$A = \frac{\partial}{\partial x}$, $B = \frac{\partial}{\partial y}$ $\qquad C = A + B$

$C\phi = \frac{\partial \varphi_1}{\partial x}\varphi_2 + \varphi_1\frac{\partial \varphi_2}{\partial y}$

$C\phi = A \otimes I_y + I_x \otimes B$

$\Rightarrow \phi = \varphi_1(x) \otimes \varphi_2(y)$

- $\vec{S} = \vec{S}_1 \otimes I_2 + I_1 \otimes \vec{S}_2$

- $s_1 = \frac{1}{2} = s_2$, baza $\qquad |\uparrow\rangle \otimes |\uparrow\rangle$, $|\uparrow\rangle \otimes |\downarrow\rangle$, $|\downarrow\rangle \otimes |\uparrow\rangle$, $|\downarrow\rangle \otimes |\downarrow\rangle$

$m \to \uparrow, \downarrow$

- $S_z = S_{1z} \otimes I_2 + I_1 \otimes S_{2z}$

$S_z|m_1\rangle \otimes |m_2\rangle = S_{1z} \otimes I_2 |m_1\rangle \otimes |m_2\rangle + I_1 \otimes S_{2z}|m_1\rangle \otimes |m_2\rangle =$

$= m_1|m_1\rangle \otimes |m_2\rangle + m_2|m_1\rangle \otimes |m_2\rangle$

$= (m_1 + m_2)|m_1\rangle \otimes |m_2\rangle$ $\qquad m = -1, 0, 1$

- $[S_\alpha, S_\beta] = [S_{1\alpha} \otimes I_2 + I_1 \otimes S_{2\alpha}, S_{1\beta} \otimes I_2 + I_1 \otimes S_{2\beta}] =$

$= [S_{1\alpha} \otimes I_2, S_{1\beta} \otimes I_2] + [I_1 \otimes S_{2\alpha}, I_1 \otimes S_{2\beta}] + \underbrace{[S_{1\alpha} \otimes I_2, I_1 \otimes S_{2\beta}]}_{=0} + \underbrace{[I_1 \otimes S_{2\alpha}, S_{1\beta} \otimes I_2]}_{=0}$

$= [S_{1\alpha}, S_{1\beta}] \otimes I_2 + I_1 \otimes [S_{2\alpha}, S_{2\beta}] + 0 + 0 =$

$= i\hbar\,\varepsilon_{\alpha\beta\gamma} S_{1\gamma} \otimes I_2 + i\hbar\,\varepsilon_{\alpha\beta\gamma} I_1 \otimes S_{2\gamma}$

$= i\hbar\,\varepsilon_{\alpha\beta\gamma} S_\gamma$

$S_\gamma = S_{1\gamma} \otimes I_2 + I_1 \otimes S_{2\gamma}$

$S_\pm = S_x \pm i S_y = S_{1\pm} \otimes I_2 + I_1 \otimes S_{2\pm}$

- $\vec{S}^2|s\,m\rangle = s(s+1)\hbar^2|s\,m\rangle$

stanje dveh delcev, celotna vrtilna kol. in spin

$S_z|s\,m\rangle = m\hbar|s\,m\rangle$

$m = m_1 + m_2 = \{-1, 0, 1\} \to s = 0$ ali 1

$|sm\rangle = ?$

$|sm\rangle$ razvijemo po bazi

$$|sm\rangle = \sum_{m_1 m_2} c_{m_1 m_2} \underbrace{|m_1\rangle \otimes |m_2\rangle}_{\substack{|m_1\rangle |m_2\rangle \\ |m_1\, m_2\rangle}}$$

poenostavitev zapisa

$|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$

$m = m_1 + m_2 \Rightarrow s = 0$ ali 1

ⓐ $s = 1$

$$S^2 |1m\rangle = 1(1+1)\hbar^2 |1m\rangle = 2\hbar^2 |1m\rangle$$

$$S_z |11\rangle = \hbar |11\rangle = \hbar |\uparrow\uparrow\rangle$$

$$|sm\rangle = |11\rangle = |\uparrow\rangle \otimes |\uparrow\rangle = \underline{1 |\uparrow\uparrow\rangle}$$

$$S_- |11\rangle = \sqrt{s(s+1) - m(m-1)}\,\hbar\, |10\rangle = \sqrt{1\cdot 2 - 0}\,\hbar\, |10\rangle = \sqrt{2}\hbar |10\rangle$$

na dva načina izračunamo ter primerjamo

$S_- |\uparrow\rangle = \hbar |\downarrow\rangle$
$S_- |\downarrow\rangle = 0$
$S_+ |\uparrow\rangle = 0$
$S_+ |\downarrow\rangle = \hbar |\uparrow\rangle$

$$S_- |\uparrow\uparrow\rangle = (S_{1-} \otimes I_2 + I_1 \otimes S_{2-}) \underbrace{|\uparrow\uparrow\rangle}_{|\uparrow\rangle \otimes |\uparrow\rangle} = S_{1-} \otimes I_2 |\uparrow\uparrow\rangle + I_1 \otimes S_{2-} |\uparrow\uparrow\rangle$$

$$= \hbar |\downarrow\rangle |\uparrow\rangle + \hbar |\uparrow\rangle |\downarrow\rangle = \hbar \left(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle \right) = \hbar \sqrt{2} |10\rangle$$

$$\Rightarrow \quad |10\rangle = \underline{\frac{1}{\sqrt{2}} \left(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle \right)}$$

$$|1\,{-1}\rangle = |s_m\rangle = |\downarrow\downarrow\rangle$$

$s = 1$	$m = 1$	$|11\rangle = |\uparrow\uparrow\rangle$	triplet stanje
	$m = 0$	$|10\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$	
	$m = -1$	$|1\,{-1}\rangle = |\downarrow\downarrow\rangle$	
$s = 0$	$m = 0$	$|00\rangle = c_1 |\uparrow\downarrow\rangle + c_2 |\downarrow\uparrow\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$	singlet

ker vemo $\langle 10 | 00 \rangle = 0$

Primer: Heisenbergova sklopitev

Kakšna je sklopitev energije?

Klasično $\uparrow \nearrow$ $\quad H \propto \vec{p}_{m_1} \cdot \vec{p}_{m_2}$

Kvantno $\quad H = J_0\, \vec{S}_1 \vec{S}_2$

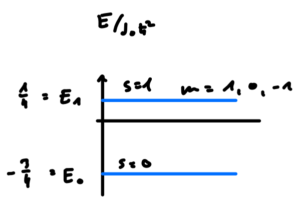
$$H |\Psi\rangle = E |\Psi\rangle \qquad \vec{S} = \vec{S}_1 + \vec{S}_2$$

$$\vec{S}^2 = (\vec{S}_1 + \vec{S}_2)(\vec{S}_1 + \vec{S}_2) = S_1^2 + S_2^2 + 2\vec{S}_1 \vec{S}_2$$

$S_1^2 = S_2^2 = \frac{1}{2}\left(\frac{1}{2}+1\right)\hbar^2 = \frac{3}{4}\hbar^2$ ∵ komutirata

$$H = \frac{J_0}{2} \left(\vec{S}^2 - \frac{3}{2}\hbar^2 \right)$$

$$H |sm\rangle = \frac{J_0 \hbar^2}{2} \left(s(s+1) - \frac{3}{2} \right) |sm\rangle \qquad E_s = J_0 \hbar^2 \begin{cases} \frac{1}{4} & s = 1 \\ -\frac{3}{4} & s = 0 \end{cases}$$



34. CLEBSCH-GORDAN COEFFICIENTS, SPHERICAL HARMONICS, AND d FUNCTIONS

Note: A square-root sign is to be understood over *every* coefficient, *e.g.*, for $-8/15$ read $-\sqrt{8/15}$.

Notation:

	J	J	...
	M	M	...
m_1 m_2			
m_1 m_2	Coefficients		
. .			

koefficient

s_1 s_2

ℓ s

← j

← m

1/2 × 1/2

	1		
	+1		
+1/2 +1/2	1		
	1	0	
	0	0	
+1/2 −1/2	1/2	1/2	
−1/2 +1/2	1/2	−1/2	
			1
			−1
−1/2 −1/2			1

1 × 1/2

	3/2		
	+3/2		
+1 +1/2	1		
	3/2	1/2	
	+1/2	+1/2	
+1 −1/2	1/3	2/3	
0 +1/2	2/3	−1/3	
	3/2	1/2	
	−1/2	−1/2	
0 −1/2	2/3	1/3	
−1 +1/2	1/3	−2/3	
	3/2		
	−3/2		
−1 −1/2	1		

2 × 1

	3		
	+3		
+2 +1	1		
	3	2	
	+2	+2	
+2 0	1/3	2/3	
+1 +1	2/3	−1/3	
	3	2	1
	+1	+1	+1
+2 −1	1/15	1/3	3/5
+1 0	8/15	1/6	−3/10
0 +1	2/5	−1/2	1/10
	3	2	1
	0	0	0
+1 −1	1/5	1/2	3/10
0 0	3/5	0	−2/5
−1 +1	1/5	−1/2	3/10
	3	2	1
	−1	−1	−1
0 −1	2/5	1/2	1/10
−1 0	8/15	−1/6	−3/10
−2 +1	1/15	−1/3	3/5
	3	2	
	−2	−2	
−1 −1	2/3	1/3	
−2 0	1/3	−2/3	
	3		
	−3		
−2 −1	1		

1 × 1

	2		
	+2		
+1 +1	1		
	2	1	
	+1	+1	
+1 0	1/2	1/2	
0 +1	1/2	−1/2	
	2	1	0
	0	0	0
+1 −1	1/6	1/2	1/3
0 0	2/3	0	−1/3
−1 +1	1/6	−1/2	1/3
	2	1	
	−1	−1	
0 −1	1/2	1/2	
−1 0	1/2	−1/2	
	2		
	−2		
−1 −1	1		

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_1^1 = -\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}$$

$$Y_2^0 = \sqrt{\frac{5}{4\pi}}\Big(\frac{3}{2}\cos^2\theta - \frac{1}{2}\Big)$$

$$Y_2^1 = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{i\phi}$$

$$Y_2^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\, e^{2i\phi}$$

2 × 1/2

	5/2		
	+5/2		
+2 +1/2	1		
	5/2	3/2	
	+3/2	+3/2	
+2 −1/2	1/5	4/5	
+1 +1/2	4/5	−1/5	
	5/2	3/2	
	+1/2	+1/2	
+1 −1/2	2/5	3/5	
0 +1/2	3/5	−2/5	
	5/2	3/2	
	−1/2	−1/2	
0 −1/2	3/5	2/5	
−1 +1/2	2/5	−3/5	
	5/2	3/2	
	−3/2	−3/2	
−1 −1/2	4/5	1/5	
−2 +1/2	1/5	−4/5	
	5/2		
	−5/2		
−2 −1/2	1		

3/2 × 1/2

	2		
	+2		
+3/2 +1/2	1		
	2	1	
	+1	+1	
+3/2 −1/2	1/4	3/4	
+1/2 +1/2	3/4	−1/4	
	2	1	
	0	0	
+1/2 −1/2	1/2	1/2	
−1/2 +1/2	1/2	−1/2	
	2	1	
	−1	−1	
−1/2 −1/2	3/4	1/4	
−3/2 +1/2	1/4	−3/4	
	2		
	−2		
−3/2 −1/2	1		

3/2 × 1

	5/2		
	+5/2		
+3/2 +1	1		
	5/2	3/2	
	+3/2	+3/2	
+3/2 0	2/5	3/5	
+1/2 +1	3/5	−2/5	
	5/2	3/2	1/2
	+1/2	+1/2	+1/2
+3/2 −1	1/10	2/5	1/2
+1/2 0	3/5	1/15	−1/3
−1/2 +1	3/10	−8/15	1/6
	5/2	3/2	1/2
	−1/2	−1/2	−1/2
+1/2 −1	3/10	8/15	1/6
−1/2 0	3/5	−1/15	−1/3
−3/2 +1	1/10	−2/5	1/2
	5/2	3/2	
	−3/2	−3/2	
−1/2 −1	3/5	2/5	
−3/2 0	2/5	−3/5	
	5/2		
	−5/2		
−3/2 −1	1		

$$\langle j_1 j_2 m_1 m_2 | j_1 j_2 J M\rangle = (-1)^{J-j_1-j_2}\langle j_2 j_1 m_2 m_1 | j_2 j_1 J M\rangle$$

$$Y_\ell^{-m} = (-1)^m Y_\ell^{m*}$$

$$d^\ell_{m,0} = \sqrt{\frac{4\pi}{2\ell+1}}\, Y_\ell^m\, e^{-im\phi}$$

$$d^j_{m',m} = (-1)^{m-m'} d^j_{m,m'} = d^j_{-m,-m'}$$

$$d^1_{0,0} = \cos\theta \qquad d^{1/2}_{1/2,1/2} = \cos\frac{\theta}{2} \qquad d^1_{1,1} = \frac{1+\cos\theta}{2}$$

$$d^{1/2}_{1/2,-1/2} = -\sin\frac{\theta}{2} \qquad d^1_{1,0} = -\frac{\sin\theta}{\sqrt{2}}$$

$$d^1_{1,-1} = \frac{1-\cos\theta}{2}$$

3/2 × 3/2

	3			
	+3			
+3/2 +3/2	1			
	3	2		
	+2	+2		
+3/2 +1/2	1/2	1/2		
+1/2 +3/2	1/2	−1/2		
	3	2	1	
	+1	+1	+1	
+3/2 −1/2	1/5	1/2	3/10	
+1/2 +1/2	3/5	0	−2/5	
−1/2 +3/2	1/5	−1/2	3/10	
	3	2	1	0
	0	0	0	0
+3/2 −3/2	1/20	1/4	9/20	1/4
+1/2 −1/2	9/20	1/4	−1/20	−1/4
−1/2 +1/2	9/20	−1/4	−1/20	1/4
−3/2 +3/2	1/20	−1/4	9/20	−1/4
	3	2	1	
	−1	−1	−1	
+1/2 −3/2	1/5	1/2	3/10	
−1/2 −1/2	3/5	0	−2/5	
−3/2 +1/2	1/5	−1/2	3/10	
	3	2		
	−2	−2		
−1/2 −3/2	1/2	1/2		
−3/2 −1/2	1/2	−1/2		
	3			
	−3			
−3/2 −3/2	1			

2 × 3/2

	7/2			
	+7/2			
+2 +3/2	1			
	7/2	5/2		
	+5/2	+5/2		
+2 +1/2	3/7	4/7		
+1 +3/2	4/7	−3/7		
	7/2	5/2	3/2	
	+3/2	+3/2	+3/2	
+2 −1/2	1/7	16/35	2/5	
+1 +1/2	4/7	1/35	−2/5	
0 +3/2	2/7	−18/35	1/5	
	7/2	5/2	3/2	1/2
	+1/2	+1/2	+1/2	+1/2
+2 −3/2	1/35	6/35	2/5	2/5
+1 −1/2	12/35	5/14	0	−3/10
0 +1/2	18/35	−3/35	−1/5	1/5
−1 +3/2	4/35	−27/70	2/5	−1/10
	7/2	5/2	3/2	1/2
	−1/2	−1/2	−1/2	−1/2
+1 −3/2	4/35	27/70	2/5	1/10
0 −1/2	18/35	3/35	−1/5	−1/5
−1 +1/2	12/35	−5/14	0	3/10
−2 +3/2	1/35	−6/35	2/5	−2/5
	7/2	5/2	3/2	
	−3/2	−3/2	−3/2	
0 −3/2	2/7	18/35	1/5	
−1 −1/2	4/7	−1/35	−2/5	
−2 +1/2	1/7	−16/35	2/5	
	7/2	5/2		
	−5/2	−5/2		
−1 −3/2	4/7	3/7		
−2 −1/2	3/7	−4/7		
	7/2			
	−7/2			
−2 −3/2	1			

2 × 2

	4				
	+4				
+2 +2	1				
	4	3			
	+3	+3			
+2 +1	1/2	1/2			
+1 +2	1/2	−1/2			
	4	3	2		
	+2	+2	+2		
+2 0	3/14	1/2	2/7		
+1 +1	4/7	0	−3/7		
0 +2	3/14	−1/2	2/7		
	4	3	2	1	
	+1	+1	+1	+1	
+2 −1	1/14	3/10	3/7	1/5	
+1 0	3/7	1/5	−1/14	−3/10	
0 +1	3/7	−1/5	−1/14	3/10	
−1 +2	1/14	−3/10	3/7	−1/5	
	4	3	2	1	0
	0	0	0	0	0
+2 −2	1/70	1/10	2/7	2/5	1/5
+1 −1	8/35	2/5	1/14	−1/10	−1/5
0 0	18/35	0	−2/7	0	1/5
−1 +1	8/35	−2/5	1/14	1/10	−1/5
−2 +2	1/70	−1/10	2/7	−2/5	1/5
	4	3	2	1	
	−1	−1	−1	−1	
+1 −2	1/14	3/10	3/7	1/5	
0 −1	3/7	1/5	−1/14	−3/10	
−1 0	3/7	−1/5	−1/14	3/10	
−2 +1	1/14	−3/10	3/7	−1/5	
	4	3	2		
	−2	−2	−2		
0 −2	3/14	1/2	2/7		
−1 −1	4/7	0	−3/7		
−2 0	3/14	−1/2	2/7		
	4	3			
	−3	−3			
−1 −2	1/2	1/2			
−2 −1	1/2	−1/2			
	4				
	−4				
−2 −2	1				

$$d^{3/2}_{3/2,3/2} = \frac{1+\cos\theta}{2}\cos\frac{\theta}{2}$$

$$d^{3/2}_{3/2,1/2} = -\sqrt{3}\,\frac{1+\cos\theta}{2}\sin\frac{\theta}{2} \qquad d^2_{2,2} = \Big(\frac{1+\cos\theta}{2}\Big)^2$$

$$d^{3/2}_{3/2,-1/2} = \sqrt{3}\,\frac{1-\cos\theta}{2}\cos\frac{\theta}{2} \qquad d^2_{2,1} = -\frac{1+\cos\theta}{2}\sin\theta$$

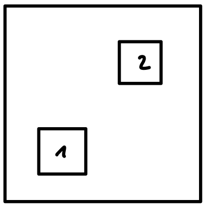
$$d^{3/2}_{3/2,-3/2} = -\frac{1-\cos\theta}{2}\sin\frac{\theta}{2} \qquad d^2_{2,0} = \frac{\sqrt{6}}{4}\sin^2\theta \qquad d^2_{1,1} = \frac{1+\cos\theta}{2}(2\cos\theta-1)$$

$$d^{3/2}_{1/2,1/2} = \frac{3\cos\theta-1}{2}\cos\frac{\theta}{2} \qquad d^2_{2,-1} = -\frac{1-\cos\theta}{2}\sin\theta \qquad d^2_{1,0} = -\sqrt{\frac{3}{2}}\sin\theta\cos\theta$$

$$d^{3/2}_{1/2,-1/2} = -\frac{3\cos\theta+1}{2}\sin\frac{\theta}{2} \qquad d^2_{2,-2} = \Big(\frac{1-\cos\theta}{2}\Big)^2 \qquad d^2_{1,-1} = \frac{1-\cos\theta}{2}(2\cos\theta+1) \qquad d^2_{0,0} = \Big(\frac{3}{2}\cos^2\theta - \frac{1}{2}\Big)$$

Figure 34.1: The sign convention is that of Wigner (*Group Theory*, Academic Press, New York, 1959), also used by Condon and Shortley (*The Theory of Atomic Spectra*, Cambridge Univ. Press, New York, 1953), Rose (*Elementary Theory of Angular Momentum*, Wiley, New York, 1957), and Cohen (*Tables of the Clebsch-Gordan Coefficients*, North American Rockwell Science Center, Thousand Oaks, Calif., 1974). The coefficients here have been calculated using computer programs written independently by Cohen and at LBNL.

Clebsch Gordonovi koeficienti



2 osjekta
z vrt. kol.

$\vec{J}_1^2, \; J_{1z}$ Velja $[J_{n\alpha}, J_{\bar{n}\beta}] = i\hbar\, \varepsilon_{\alpha\beta\gamma}\, \delta_{n\bar{n}}\, S_{n\gamma}$

$\vec{J}_2^2, \; J_{2z}$ $\vec{J} = \vec{J}_1 \otimes I_2 + I_1 \otimes \vec{J}_2 \equiv \vec{J}_1 + \vec{J}_2$

$\vec{J}_1 \overset{\text{je lahko}}{=} \vec{L}_1, \vec{S}_1, \vec{J}_1, \dots$

Baza $\quad |j_1 m_1\rangle \otimes |j_2 m_2\rangle = |j_1 m_1 j_2 m_2\rangle$

$(2j_1+1)(2j_2+1)$ ... baznih vektorjev

Npr. $\vec{J}_1 = \vec{L}, \; \vec{J}_2 = \vec{S} \quad (2l+1)\cdot 2$

$|j\,m\rangle \equiv |j_1 j_2\; j\, m\rangle$

skupna baza

$$|j_1 j_2\; j\, m\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} |j_1 m_1\rangle |j_2 m_2\rangle \underbrace{\langle j_1 m_1 j_2 m_2 | j\, m\rangle}_{\text{koeficient razvoja}}$$

Clebsch Gordonov koeficient $C^{jm}_{j_1 m_1 j_2 m_2}$

$C \neq 0$ kadar $m = m_1 + m_2 \quad |j_1 - j_2| \leq j \leq j_1 + j_2$

Primer uporabe tabele

$l = 1 \quad s = \frac{1}{2}$

$l \times s$: $1\times 1/2$

		3/2	
		+3/2	
+1	+1/2	1	
		3/2	1/2
		+1/2	+1/2
+1	−1/2	1/3	2/3
0	+1/2	2/3	−1/3

$|j\,m\rangle = ?$

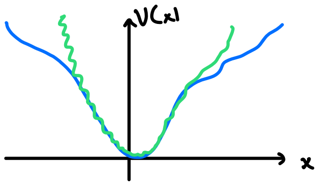
dobimo iz izbirnih pravil

s tabelo $\; j = \frac{1}{2} \;\; m = \frac{1}{2} \qquad \Psi = \sqrt{\frac{2}{3}} \begin{pmatrix} 0 \\ Y_1^1 \end{pmatrix} - \sqrt{\frac{1}{3}} \begin{pmatrix} Y_1^0 \\ 0 \end{pmatrix}$

$$|j_1 j_2 j\, m\rangle = |1\, \tfrac{1}{2}\, \tfrac{1}{2}\, \tfrac{1}{2}\rangle = \sqrt{\tfrac{2}{3}}\,|1\,1\rangle |\tfrac{1}{2}\, -\tfrac{1}{2}\rangle - \sqrt{\tfrac{1}{3}}\,|1\,0\rangle |\tfrac{1}{2}\, \tfrac{1}{2}\rangle$$

Teorija motenj (perturbacij)

Rayleigh-Schrödingerjeva metoda (nedegeneriran spekter)



$$H = \underbrace{\tfrac{1}{2}kx^2}_{} + \underbrace{\alpha x^3 + \beta x^4 + \dots}_{H_1 = \lambda \hat{V}} + \underbrace{\tfrac{p^2}{2m}}_{H_0}$$

$H = H_0 + H_1$

$H_0 |n^0\rangle = E^{(0)} |n^0\rangle$ poznamo rešitve za H_0

$\langle m^0 | n^0\rangle = \delta_{mn}$ ortonormirane, nedegenerirana

Iščemo $\quad H|n\rangle = E_n |n\rangle$ popravki

$|n\rangle = |n^0\rangle + \lambda |n^1\rangle + \lambda^2 |n^2\rangle + \dots \qquad \lambda$ ... brezdim. parameter

ne sme biti 0 $\quad E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots$

Predpostavka $\quad 0 \neq \langle n^0 | n\rangle = 1 + \lambda \langle n^0 | n^1\rangle + \lambda^2 \langle n^0 | n^2\rangle + \dots \equiv 1$

kasneje bomo renormirali funkcijo $\quad \Rightarrow \langle n^0 | n^i\rangle = 0 \qquad i = 1, 2, \dots \quad \forall \lambda$

$$(H_0 + \lambda V)(|n^0\rangle + \lambda|n^1\rangle + \dots) = (E_n^{(0)} + \lambda E_n^{(1)} + \dots)(|n^0\rangle + \lambda|n^1\rangle + \dots)$$

λ^0 : $H_0|n^0\rangle = E_n^{(0)}|n^0\rangle$ ✓

λ^1 : $H_0|n^1\rangle + V|n^0\rangle = E_n^{(1)}|n^0\rangle + E_n^{(0)}|n^1\rangle$ $\quad /\langle n^0|$

λ^2 : $H_0|n^2\rangle + V|n^1\rangle = E_n^{(0)}|n^2\rangle + E_n^{(1)}|n^1\rangle + E_n^{(2)}|n^0\rangle$

$\vdots$

λ^1 $\quad \underbrace{\langle n^0|H_0|n^1\rangle}_{E_n^{(0)}\langle n^0|n^1\rangle = 0} + \underbrace{\langle n^0|V|n^0\rangle}_{V_{nn}} = E_n^{(1)} + 0$ matrični element

$$\Rightarrow \boxed{E_n^{(1)} = V_{nn}}$$

$|m\rangle$ je baza nezmotenega problema (H_0)

$$I = \sum_m |m^0\rangle\langle m^0|$$

$H_0|m\rangle = E_n|m\rangle$

$$|n^1\rangle = I|n^1\rangle = \sum_{m\neq n}|m^0\rangle\underbrace{\langle m^0|n^1\rangle}_{?}$$

Vstavimo pri λ^1 in pomnožimo z $\langle m^0|$

$$\lambda^1: \underbrace{\langle m^0|H_0|n^1\rangle}_{E_m^{(0)}\langle m^0|n^1\rangle} + \underbrace{\langle m^0|V|n^0\rangle}_{V_{mn}} = E_n^{(0)}\langle m^0|n^1\rangle + E_n^{(1)}\underbrace{\langle m^0|n^0\rangle}_{=0}$$

$$\langle m^0|n^1\rangle = \frac{V_{mn}}{E_n^{(0)} - E_m^{(0)}}$$

$$\Rightarrow \boxed{|n^1\rangle = \sum_{m\neq n}\frac{V_{mn}}{E_n^{(0)} - E_m^{(0)}}|m^0\rangle}$$

λ^2 : Pomnožimo z $\langle n^0|$ $\Rightarrow$ $\boxed{E_n^{(2)} = \langle n^0|V|n^1\rangle = \sum_{m\neq n}\frac{|V_{mn}|^2}{E_n^{(0)} - E_m^{(0)}}}$

Rezultat v 2. redu

$$\boxed{\begin{aligned} E_n &= E_n^{(0)} + \lambda\underbrace{V_{nn}}_{E_n^{(1)}} + \lambda^2\underbrace{\sum_{m\neq n}\frac{|V_{mn}|^2}{E_n^{(0)} - E_m^{(0)}}}_{E_n^{(2)}} + \mathcal{O}(\lambda^3) \\ |n\rangle &= |n^0\rangle + \lambda\sum_{m\neq n}\frac{V_{mn}}{E_n^{(0)} - E_m^{(0)}}|m^0\rangle + \mathcal{O}(\lambda^2)\end{aligned}} \qquad \lambda \to 1$$

Renormalizacija

$$\langle n|n\rangle = (\langle n^0| + \lambda\langle n^1| + \mathcal{O}(\lambda^2))(|n^0\rangle + \lambda|n^1\rangle + \mathcal{O}(\lambda^2)) = 1 + \mathcal{O}(\lambda^2)$$

Naj bo $E_n^{(0)}$ osnovno stanje, n. Torej je $E_n^{(0)} < E_m^{(0)}$ za $\forall m$, od koder sledi $E_n^{(2)} < 0$

Degeneriran spekter

$H = H_0 + \lambda V$

H_0 je 2x degeneriran

$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots$

funkciji pri degenerirani energiji

$$|n\rangle = \underbrace{c_1|n_1^0\rangle + c_2|n_2^0\rangle}_{|n^0\rangle \text{ ker je degeneriran}} + \lambda|n^1\rangle + \dots$$

$H|n\rangle = E_n|n\rangle$

$(H_0 + \lambda V)|n\rangle = E_n|n\rangle$

λ^0: $H_0|n_1^0\rangle = E_n^{(0)}|n_1^0\rangle$

$H_0|n_2^0\rangle = E_n^{(0)}|n_2^0\rangle$

λ^1: $H_0|n^1\rangle + c_1 V|n_1^0\rangle + c_2 V|n_2^0\rangle = E_n^{(0)}|n^1\rangle + E_n^{(1)}\left(c_1|n_1^0\rangle + c_2|n_2^0\rangle\right)$

$\langle n_1^0|/$ $\quad \underbrace{\langle n_1^0|H_0|n^1\rangle}_{=0} + c_1\underbrace{\langle n_1^0|V|n_1^0\rangle}_{=V_{11}} + c_2\underbrace{\langle n_1^0|V|n_2^0\rangle}_{=V_{12}} = E_n^{(0)}\underbrace{\langle n_1^0|n^1\rangle}_{=0} + E_n^{(1)}\left(c_1\underbrace{\langle n_1^0|n_1^0\rangle}_{=1} + c_2\underbrace{\langle n_1^0|n_2^0\rangle}_{=0}\right)$

$$V_{11}c_1 + V_{12}c_2 = E_n^{(1)}c_1$$

$\langle n_2^0|/$ $\quad \underbrace{\langle n_2^0|H_0|n^1\rangle}_{=0} + c_1\underbrace{\langle n_2^0|V|n_1^0\rangle}_{=V_{21}} + c_2\underbrace{\langle n_2^0|V|n_2^0\rangle}_{=V_{22}} = E_n^{(0)}\underbrace{\langle n_2^0|n^1\rangle}_{=0} + E_n^{(1)}\left(c_1\underbrace{\langle n_2^0|n_1^0\rangle}_{=0} + c_2\underbrace{\langle n_2^0|n_2^0\rangle}_{=1}\right)$

$$V_{21}c_1 + V_{22}c_2 = E_n^{(1)}c_2$$

$$\Rightarrow \quad \begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix}\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = E_n^{(1)}\begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$

$\Rightarrow$ Dobimo dve rešitvi (kot odmik v mag polju osn. stanja H zaradi spina)

Omejitve

- vrsta perturbacij divergira
  - $H = \frac{p^2}{2m} + \frac{kx^2}{2} + \underbrace{\lambda x}_{\text{perturbacija}}$ (premaknjen oscilator) ima analitično rešitev $\forall \lambda \in \mathbb{R}$

    $\lambda_R = \infty$

    $E_n = E_n^0 + \sum_k c_k \lambda^k$ vrsta konvergira $|\lambda| < \lambda_R$
  - $H = \frac{p^2}{2m} + \frac{kx^2}{2} + \lambda x^2 = \frac{p^2}{2m} + \frac{k}{2}\left(1 + \frac{2\lambda}{k}\right)x^2$

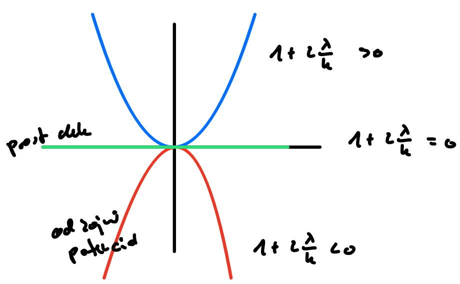
    Pri HO je $k = m\omega^2$

    $$H = \frac{p^2}{2m} + \frac{m\omega^2}{2}\left(1 + \frac{2\lambda}{m\omega^2}\right)x^2$$

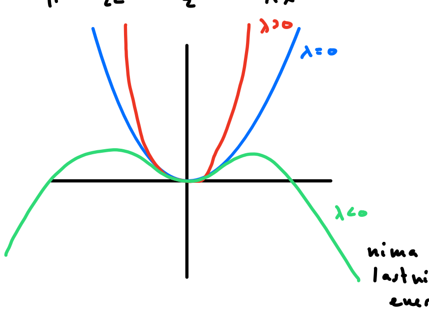
    $E_n^{(0)} = \hbar\omega\left(n + \frac{1}{2}\right)$ za naš prob. $E_n = \hbar\omega\sqrt{1 + 2\frac{\lambda}{k}}\left(n + \frac{1}{2}\right)$

    Razvijemo E_n po λ, dobimo binomsko vrsto, za katero velja $2\frac{\lambda}{k} < 1$

    $\Rightarrow$ ne konvergira za $\forall\lambda$



  - $H = \frac{p^2}{2m} + \frac{kx^2}{2} + \lambda x^4$ $\quad \lambda_R = ?$



$\Rightarrow \lambda_R = 0$

- fazni prehodi:
  - super prevodnost $\longrightarrow T_c \propto e^{-\frac{c}{\lambda}}$

Brillouin Wignerjeva perturbacija

$H = H_0 + \lambda V$

$$E_n = E_n^{(0)} + \lambda V_{nn} + \lambda^2 \sum_m \frac{|V_{mn}|^2}{E_n - E_m^{(0)}} + \lambda^j \sum_{\substack{m_1\\ m_2\\ \vdots \\ m_{j-1}}} \frac{V_{nm_1} V_{m_1 m_2} \cdots V_{m_{j-1} n}}{(E_n - E_{m_1}^{(0)})(E_n - E_{m_2}^{(0)}) \cdots (E_n - E_{m_{j-1}}^{(0)})}$$

Implicitna enačba $f(E_n) = 0$

Časovno odvisna motnja

$$H(t) = H_0 + \lambda \hat{V}(t)$$

$H_0 |n\rangle = E_n |n\rangle$ $\quad |n\rangle$ baza, $\langle n|m\rangle = \delta_{nm}$

$t = 0 \quad |\psi(0)\rangle = \sum_n c_n(0) |n\rangle$

$t > 0 \quad |\psi(t)\rangle = \sum_n c_n(t) e^{-i \frac{E_n}{\hbar} t} |n\rangle$

$$i\hbar \frac{\partial \psi}{\partial t} = H(t)\, \psi(t)$$

$$i\hbar \sum_n \left(\frac{\partial c_n}{\partial t} e^{-i \frac{E_n}{\hbar} t} \cancel{- i \frac{E_n}{\hbar} c_n e^{-i \frac{E_n}{\hbar} t}} \right) |n\rangle = \sum_n (\cancel{E_n} + \lambda V(t))\, e^{-i \frac{E_n}{\hbar} t} c_n |n\rangle \qquad / \langle m|$$

$$i\hbar \frac{\partial c_m}{\partial t} e^{-i \frac{E_m}{\hbar} t} = \lambda \sum_n \langle m | V(t) | n \rangle e^{-i \frac{E_n}{\hbar} t} c_n(t)$$

$$i\hbar \frac{\partial c_m}{\partial t} = \lambda \sum_n \underbrace{\langle m | V(t) | n \rangle e^{-i \frac{E_n - E_m}{\hbar} t}}_{V_{mn}(t)} c_n(t)$$

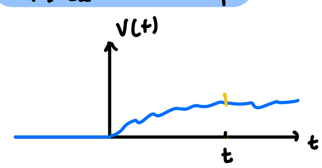
$$i\hbar \frac{\partial c_m}{\partial t} = \lambda \sum V_{mn}\, c_n(t)$$

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} c_1 \\ \vdots \\ c_m \end{pmatrix} = \lambda \begin{bmatrix} V_{11}(t) & V_{12}(t) & \\ & V_{22}(t) & \ddots & \\ & & & V_{mm}(t) \end{bmatrix} \begin{pmatrix} c_1 \\ \vdots \\ c_m \end{pmatrix}$$

$i\hbar \dot{\vec{c}} = \lambda \underline{\underline{V}}(t)\, \vec{c}$ $\quad$ (to je točno) $\quad$ Diracova slika

$\lambda = 1$

Šibka motnja



$$V(t) = \begin{cases} 0 & t < 0 \\ v(t) & t > 0 \end{cases}$$

$|\psi(0)\rangle = |m\rangle = \sum_n c_n(0) |n\rangle \;:\; c_n(0) = \delta_{nm}$

$$i\hbar \frac{\partial c_k}{\partial t} = \lambda \sum_n V_{kn}(t)\, c_n(t) = \lambda V_{km}(t) \cdot 1 \qquad \text{za } \lambda \ll 1$$

$c_m(0) = 1$

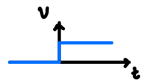
$c|_{n \neq m} = 0$

$$c_k(t) = \frac{\lambda}{i\hbar} \int^t V_{km}(t')\, dt' \qquad k \neq m$$

$c_m(t) \approx 1$ $\quad$ če $|c_k|^2 \ll 1$

Fermijevo zlato pravilo

$$V(t) = \begin{cases} 0 & t<0 \\ v & t>0 \end{cases}$$



$$\langle m|V|n\rangle = V_{mn}$$

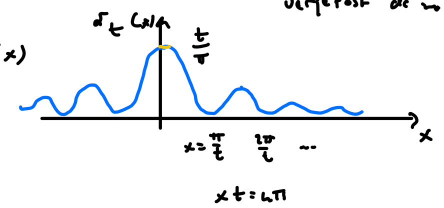
$k \neq n$ $\quad c_k(t) = \frac{1}{i\hbar}\int_0^t V_{kn}\, e^{i\frac{E_k - E_n}{\hbar}t'}\, dt' = \frac{V_{kn}}{i\hbar}\,\frac{e^{-i\omega_{kn}}-1}{-i\omega_{kn}}$ $\qquad \omega_{kn}$

$k = n$ $\quad c_n(t) = 1$

$P_{n\to m}$ $\quad P_{kn}(t) = \frac{|V_{kn}|^2}{\hbar^2}\,\frac{\sin^2 \frac{1}{2}\omega_{kn} t}{(\frac{1}{2}\omega_{kn})^2} = |c_k|^2$

P_{kn} verjetnost da se začeli v m in končali v k

$$\delta_t(x) = \frac{1}{\pi}\,\frac{\sin^2 xt}{x^2 t} \xrightarrow{t\to\infty} \delta(x)$$

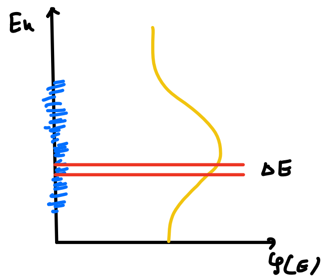


kot pri uklonski reži

$$P_{kn} = \frac{2\pi}{\hbar}|V_{kn}|^2\,\delta_t(E_k - E_n)\,t \qquad P_{kn} \ll 1 \quad t\to\infty$$

$$P_{nn} \approx 1$$

Gostota stanj



$$g(E) = \frac{\Delta N}{\Delta E} \to \frac{dN}{dE}$$

$$P_{konč} = \sum_{k\neq n} P_{kn} \to \int P_{kn}(t)\, g(E_k)\, dE_k$$

$$P = \frac{2\pi}{\hbar}|V_{kn}|^2\, g(E_n)\, t \qquad \propto t$$

Imamo delce v neki stanju, ki ima ustrezno konst. motnjo. Po dolgem času je najverjetneje, da preide nazaj v osnovno

verjetnost

$$\boxed{\frac{dP}{dt} = w = \frac{2\pi}{\hbar}|V_{kn}|^2\, g(E_n)}$$

od časa neodvisno

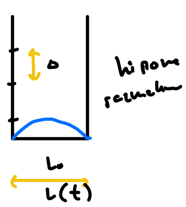
Primer: radioaktivnost

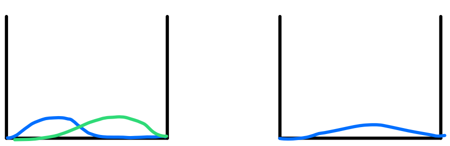
$t=0 \quad |\psi(0)\rangle$

$$-dN = N\,dP = Nw\,dt \quad \Rightarrow \quad N = N_0 e^{-wt}$$

Adiabatne spremembe in kvantne faze

$H(t)$





$L_0 \to 2L_0$
zelo počasi raztegnemo plošči
sistem bo vedno čez v osnovnem stanju

tipična frekvenca

$$\frac{dL}{dt} \ll \left(\frac{\Delta}{\hbar}\right)L$$

ω

$$\Delta = E_k - E_n$$

Kvantni sistem $H(\vec{Q}(t))$ $\qquad \vec{Q} = (L, V_0, \vec{B}, \dots) = \vec{Q}(t) = (q_1, q_2, \dots)$

odvisen od različnih parametrov

$$H(\vec{Q})|\psi_n(\vec{Q})\rangle = E_n(\vec{Q})|\psi_n(\vec{Q})\rangle$$

$$\psi_n^0(\vec{r},t) = \langle \vec{r} | \psi_n(\vec{Q}(t))\rangle$$

$$i\hbar \frac{\partial}{\partial t}|\psi_n^0\rangle \neq H(\vec{Q}(t))|\psi_n^0\rangle$$

Adiabatni režim

iščemo $\phi_n(t)$

$$|\psi_n\rangle = e^{i\phi_n(t)}|\psi_n^0\rangle$$

$$i\hbar \frac{\partial}{\partial t}|\psi_n\rangle = H|\psi_n\rangle$$

$$i\hbar\left(i\frac{d\phi_n}{dt}e^{i\phi_n}|\psi_n^0\rangle + e^{i\phi_n}\frac{\partial}{\partial t}|\psi_n^0\rangle\right) = H e^{i\phi_n}|\psi_n^0\rangle = e^{i\phi_n}E_n|\psi_n^0\rangle \qquad /\langle\psi_n^0|$$

$$i\hbar\left(i\frac{\partial\phi_n}{\partial t}\underbrace{\langle\psi_n^0|\psi_n^0\rangle}_{=1} + \langle\psi_n^0|\frac{\partial}{\partial t}|\psi_n^0\rangle\right) = E_n\underbrace{\langle\psi_n^0|\psi_n^0\rangle}_{=1}$$

$$-\hbar\frac{\partial\phi_n}{\partial t} + i\hbar\langle\psi_n^0|\frac{\partial}{\partial t}|\psi_n^0\rangle = E_n$$

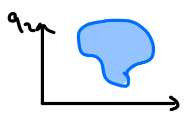
Naj bo $\phi_n = \gamma_n + \theta_n$

$$i\hbar\left(i\frac{\partial\gamma_n}{\partial t} + \langle\psi_n^0|\frac{\partial}{\partial t}|\psi_n^0\rangle\right) = E_n + \hbar\frac{\partial\theta_n}{\partial t} \underset{\substack{\uparrow\\ \text{naj bo}}}{= 0}$$

$$\Rightarrow \frac{\partial\theta_n}{\partial t} = -\frac{E_n(t)}{\hbar} \qquad \theta_n = -\frac{1}{\hbar}\int_0^t E_n(t')\,dt'$$

$$\frac{\partial\gamma_n}{\partial t} = i\langle\psi_n^0|\frac{\partial\psi_n^0}{\partial t}\rangle$$

$$\frac{\partial}{\partial t}\psi_n^0 = \sum_i \frac{\partial\psi_n^0}{\partial q_i}\dot{q}_i = (\nabla_{\vec{Q}}\psi_n^0)\dot{\vec{Q}}$$

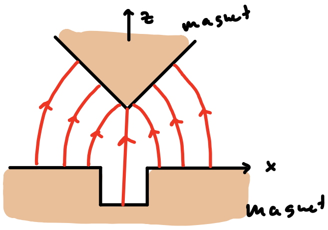


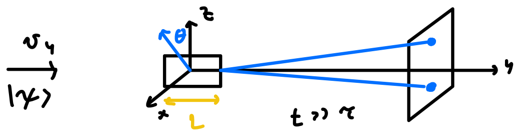
$$\gamma_n(t) = i\int_0^t \langle\psi_n^0|\vec{\nabla}_Q\psi_n^0\rangle\cdot\underbrace{\dot{\vec{Q}}\,dt}_{d\vec{Q}} = i\int_{\vec{Q}(0)}^{\vec{Q}(t)}\langle\psi_n^0|\vec{\nabla}_Q\psi_n^0\rangle\cdot d\vec{Q}$$

Berryjeva faza $\qquad \gamma_n = i\oint\langle\psi_n^0|\vec{\nabla}_Q\psi_n^0\rangle\,d\vec{Q}$

Kvantna meritev

Stern – Gerlach





- Semiklasično

$$\vec{F} = (\vec{\mu}\cdot\nabla)\vec{B}(\vec{r}) = -\nabla(-\vec{\mu}\cdot\vec{B}) = \nabla\vec{\mu}\cdot\vec{B}$$

$$\vec{B} = \vec{B}_0 + \sum_a \frac{\partial\vec{B}}{\partial x_a}\Big|_a x_a + \dots$$

$$F_z = \mu\frac{\partial B_z}{\partial z}\Big|_{z=0}$$

$$\tau = \frac{L}{v_y} \qquad p_z = \int F_z\, dt \approx \pm|F_z|\tau$$

sunek sile v z smeri

$$\chi = \begin{pmatrix}\cos\theta/2\\ \sin\theta/2\end{pmatrix}$$

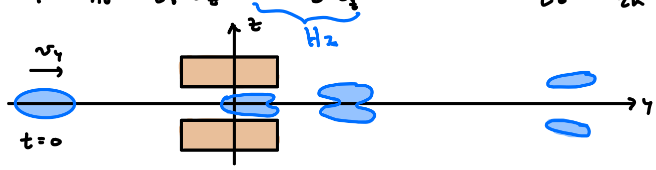
$$P_\uparrow = |\langle\uparrow|\chi\rangle|^2 = \cos^2\theta/2$$

$$P_\downarrow = |\langle\downarrow|\chi\rangle|^2 = \sin^2\theta/2 = 1 - P_\uparrow$$

- Kvantno

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e}{m}\vec{S}\cdot\vec{B} = H_0 + H_B$$

$$H = H_0 - E_0\sigma_z \underbrace{- F z\sigma_z}_{H_z} \qquad E_0 = \frac{e\hbar}{2m}B_0 \qquad F = \frac{e\hbar}{2m}\frac{\partial B_z}{\partial z}\Big|_{z=0}$$



$$\Psi(\vec{r},0) = \psi(\vec{r},0)\chi = \psi(\vec{r},0)\begin{pmatrix}\cos\theta/2\\ \sin\theta/2\end{pmatrix}$$

$$\Psi(\vec{r},t) = \psi_0(x,y,t)\begin{pmatrix}\psi_\uparrow(z,t)\\ \psi_\downarrow(z,t)\end{pmatrix}$$

$B = 0$ $$\psi(\vec{r},t) = \psi_0(x,y,t)\int_{-\infty}^{\infty}\tilde{\psi}(p)\, e^{i\frac{p}{\hbar}z - i\frac{E_p}{\hbar}t}$$

$B \neq 0$, $\tau \ll t$ $$U = e^{-i\frac{H_z}{\hbar}t} = e^{i\frac{F}{\hbar}\sigma_z t z}\Big|_{t=\tau}$$

$$U e^{i\frac{p}{\hbar}z} = e^{i\frac{p}{\hbar}z \pm i\frac{F}{\hbar}z\tau}$$

- Von Neumannova kvantna meritev

$$H = H_0 + H_{int}(q,p,t) \qquad \hat{p} = -i\hbar\frac{\partial}{\partial q} \qquad q = z$$

ⓐ $H_{int} = \frac{g}{\tau}\hat{A}\cdot\hat{p}$

ⓑ $H_{int} = -\frac{g}{\tau}\hat{A}\cdot\hat{q}$ pointer / kazalec