## Hamiltoniaan zonder spin; deeltje onder vrije val:

$$\hat H = -\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + \underbrace{V(z)}_{\text{delta/gaussisch potentiaal}} + \underbrace{mgz}_{\text{lineare grav. pot.}}$$

$\boxed{\text{Spin}}$

$$\hat H_{spin} = -\vec\mu \circ \vec B$$
$$= -\gamma \frac{\hbar}{2}\vec\sigma \circ \vec B$$

met $\gamma$ de gyromagnetisch ratio ; $\gamma = g\frac{\mu_B}{\hbar}$ voor $e^-$ (Bohr Magneton.)

- $\vec\sigma = (\sigma_x, \sigma_y, \sigma_z)$, Pauli matrices
- $\vec B$ = magnetisch veld

$$\hat H_{tot} = \underbrace{-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + V(z) + mgz}\; + \underbrace{\left(-\gamma\frac{\hbar}{2}\vec\sigma\circ\vec B\right)}_{\text{spin}}$$

$$\left\{\begin{aligned} \mu_B &= \frac{e\hbar}{2m_e} \\ &= \frac{1}{2}\frac{e\hbar}{m_e} \\ &\sim 5{,}7883 \cdot 10^{-5}\ eV/T \\ &\sim 9{,}274 \cdot 10^{-24}\ J/T \end{aligned}\right.$$

$\rightarrow B(z)$, is belangrijk.

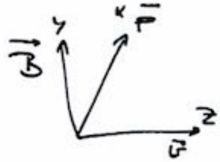
## Toepassing op Split-Operator Methode

Voor (de) split-operator methode, wordt de $\psi$ op stap $+\Delta t$ berekend:

- $$\psi(z, t+\Delta t) \approx \underbrace{e^{-i/\hbar\,\hat T \frac{\Delta t}{2}}}_{\text{kin}}\;\underbrace{e^{-i/\hbar\,\hat V \Delta t}}_{\text{pot}}\;\underbrace{e^{-i/\hbar\,\hat T \Delta t/2}}_{\text{kin}}\;\psi(z,t)$$

met $\hat T = -\frac{\hbar^2}{2m}\frac{d^2}{dz^2}$, de kinetische operator

$\hat V = +V(z) + mgz - \gamma\,\hbar/2\;\vec\sigma\circ\vec B$.




* Neem $\vec B$ in y-richting, $\vec\sigma\circ\vec B$ wordt $\boxed{\sigma_y B_y}$

* Berekening op aparte spincomponenten:

$$\boxed{\hat H = \hat T + \hat V}$$

$$\psi(z,t) = \begin{pmatrix}\psi_\uparrow(z,t)\\ \psi_\downarrow(z,t)\end{pmatrix}$$

$$\psi(z,t+\Delta t) \approx e^{-i/\hbar \hat{T}\frac{\Delta t}{2}} e^{-i/\hbar \hat{V}\Delta t} e^{-i/\hbar \hat{T}\frac{\Delta t}{2}} \psi(z,t)$$

## $\boxed{\text{Split-operator Methode}}$

$$\hat{H}_{tot} = \underbrace{-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}}_{\hat{H}_{kin}} + \underbrace{V(z) + mgz - \gamma\, \hbar/2\, \sigma B(z)}_{\hat{H}_{pot}}$$

For general simulation, assume general solution:

$$\psi(z,t+dt) = e^{-\frac{i\hat{H}dt}{\hbar}} \psi(z,t+dt)$$

$$= e^{-\frac{i}{\hbar}\hat{H}_{kin}dt} e^{\frac{-i}{\hbar}\hat{H}_{pot}dt} \psi(z,t+dt)$$

$\hat{H}_{kin}$ & $\hat{H}_{pot}$ commuteren niet

Gebruik BCH-formule voor non-commuterende operatoren $\boxed{\text{Baker-Campbell-Hausdorff}}$

$$e^X e^Y = e^Z, \text{ dan } Z = X + Y + \frac{1}{2}[X,Y] + \frac{1}{12}[X,[X,Y]] - \frac{1}{12}$$

dus $\boxed{e^X e^Y = e^X e^Y e^{\frac{1}{2}[X,Y]}}$

$$\psi(\vec{r},t+dt) = \left[e^{\frac{-i}{\hbar}\hat{H}_{kin}dt} e^{\frac{-i}{\hbar}\hat{H}_{pot}dt} e^{-\frac{i}{\hbar 2}[\hat{H}_{kin},\hat{H}_{pot}]dt^2}\right]\psi(\vec{r},t)$$

*

$\boxed{dt^2 \text{ error}}$

$\Rightarrow$ Gebruik $\boxed{\text{Strang splitting}}$ om error $dt^2$ → $dt^3$ te krijgen

$$\psi(\vec{r},t+dt) = \left[e^{-i/\hbar \hat{H}_{pot}\frac{dt}{2}} e^{-i/\hbar \hat{H}_{kin}dt} e^{-i/\hbar \hat{H}_{pot.}dt/2}\right]\psi(\vec{r},t) + \mathcal{O}(dt^3)$$

→ [pot halfstap (iFFT) → FFT pot half stap

# Strang Splitting

Consider $\dot{y} = L_1(y) + L_2(y)$, when $L_1/L_2$ are operators.

~~[illegible]~~ with associated solution $y(t) = e^{(L_1+L_2)t} y_0$

if $L_1$ and $L_2$ commute, then by exp. laws, this is equivalent to:

$$y(t) = e^{L_1 t} e^{L_2 t} y_0.$$

if $L_1$ and $L_2$ don't commute, then.

$$e^{(L_1+L_2)t} y_0 = e^{L_1 t} e^{L_2 t} y_0 + O(t^2)$$

with error $t^2$, we now have:

$$1^{st} \left| \begin{aligned} \tilde{y}_1 &= e^{L_1 \Delta t} y_0 \\ y_1 &= e^{L_2 \Delta t} \tilde{y}_1 \end{aligned} \right.$$

$$2^{nd} \left| \begin{aligned} \tilde{y}_2 &= e^{L_1 \Delta t} y_1 \\ y_2 &= e^{L_2 \Delta t} \tilde{y}_2 \end{aligned} \right.$$

$\vdots$

we can extend this approach to second order $[O(t^3)]$, by taking half-steps:

$$1^{st}\,\text{step} \left| \begin{aligned} \tilde{y}_1 &= e^{L_1 \Delta t/2} y_0 \\ \overline{y_1} &= e^{L_2 \Delta t} \tilde{y}_1 \\ y_1 &= e^{L_1 \Delta t/2} \overline{y_1} \end{aligned} \right.$$

$$2^{nd} \left| \begin{aligned} \tilde{y}_2 &= e^{L_1 \Delta t/2} y_1 \\ \overline{y_2} &= e^{L_2 \Delta t} \tilde{y}_2 \\ y_2 &= e^{L_1 \Delta t/2} \overline{y_2} \end{aligned} \right.$$

we can prove that Strang splitting is of second order by

1) using BCH
2) Rooted tree Analysis
3) Taylor Expansion & comparing error terms

Defining an absorption mask & calculating probability loss

* $\Psi(z) = \psi_{Re}(z) = i\,\psi_{Im}(z)$

with local probability:

$$|\psi(z)|^2 = \psi_{Re}^2(z) + \psi_{Im}^2(z)$$

* Apply Mask $M(z)$:

$$\psi'(z) = M(z)\,\psi(z),$$

with $M(z)$ : $\begin{cases} 1 , & x_{min} - \text{margin} \leq z \leq x_{max} - \text{margin} \\ e^{-\left(\frac{x_{min} - \text{margin} - z}{\text{margin}}\right)^2} & z < x_{min} - \text{margin} \\ e^{-\left(\frac{z - (x_{max} + \text{margin})}{\text{margin}}\right)^2} & z > x_{max} + \text{margin} \end{cases}$

the updated probability density is

$$|\psi'(z)|^2 = \cancel{M} \, m(z)^2 \, |\psi(z)|^2$$

→ local proability loss at each point:

$$\Delta P_{lost}(z) = |\psi(z)|^2 - |\psi'(z)|^2 = \left(1 - m(z)^2\right) |\psi(z)|^2$$

Continuous → 1) $\Delta P_{lost}(z)_{Total} = \int \left(1 - M^2(z)\right) |\psi(z)|^2 \, dz$

discrete → 2) $\Delta P_{lost\,total}(z) = \sum_i \left(1 - M^2(z_i)\right) |\psi(z_i)|^2 \, \Delta z,$

with $\Delta z$ the spacing between points.

and so we do the following: $\psi(r,t)$

$$e^{-i/\hbar \hat{H}_{pot}\, dt/2}\, \psi(r,t)$$

FFT

$$\times e^{-i/\hbar \hat{H}_{kin}\, dt}\, \psi(r,t)$$

IFFT

$$e^{-i/\hbar \hat{H}_{pot}\, dt/2}\, \psi(r,t)$$

$\psi(r, t+dt)$

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Now for introducing spin into this equation:

$$\hat{H}_{pot} = V(z) + mgz - \gamma\, \hbar/2\, \vec{\sigma} \cdot \vec{B}$$