$(\hbar = 1)$

$$i\hbar\dot{\psi} = \Big[\underbrace{\frac{-\hbar^2}{2m}\nabla^2}_{} + \underbrace{V(\vec r) + g|\psi(\vec r)|^2}_{H_p(\vec r)}\Big]\psi(\vec r) = (\hat H_k + \hat H_p)\psi(\vec r)$$

$$\hat H_k = \frac{\hbar^2 k^2}{2m}$$

$\psi(t) \longrightarrow \psi(\vec r, t+\Delta t)$

$\psi(x) \xrightarrow{FFT} \Phi(k)$

$$\psi(t+\Delta t) = e^{i\hat H \Delta t}\psi(t) \cong e^{i\hat H_k \Delta t}\,\underbrace{e^{i\hat H_p \Delta t}\psi(\vec r, t)}$$

$$\underbrace{e^{i[V(\vec r) + g|\psi(\vec r,t)|^2]t}\,\psi(\vec r, t)}$$

$$\tilde\Psi(\vec r) \xrightarrow{F.F.T.(3D)} \tilde\Phi(\vec k)$$

$$e^{i\frac{\hbar^2 k^2}{2m}\Delta t}\,\tilde\Phi(\vec k) = \eta(\vec k) \xrightarrow{(FFT)^{-1}} \psi(t+\Delta t)$$

② $$\boxed{\psi(t+\Delta t) = FFT^{(-1)}\Big[e^{i\frac{\hbar k^2}{2m}\Delta t}\,FFT\Big[e^{i[V(\vec r) + g|\psi(\vec r,t)|^2]\Delta t}\,\psi(\vec r,t)\Big]\Big]}$$

$-i$ $\quad 2$ $\quad -i$ $\quad 2$

$RZE \to u = 1i$

$IZE \to u = -1$

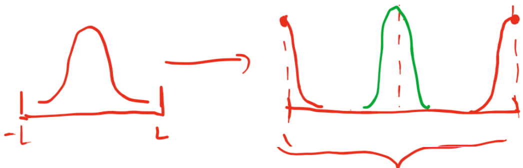
$$\int |\psi(\vec r,t)|^2\, d^3\vec r = 1$$

• DDWW $\longrightarrow g|\psi(\vec r)|^2 + \int d^3r'\, V(\vec r - \vec r')\,|\psi(\vec r')|^2$

$$\underbrace{\int \frac{d^3k}{(2\pi)^3}}_{FFT^{-1}} e^{i\vec k\cdot\vec r}\,\tilde V(\vec k)\,\tilde n(\vec k) \quad \tilde n(\vec k) \to FT\left[|\psi(\vec r)|^2\right]$$

$$\tilde V(\vec k) \to \frac{4\pi}{3}\left(3\frac{k_z^2}{k^2} - 1\right)$$

① • FFT (1D): $\psi(x) \longrightarrow \phi(k)$



FFT

$$\frac{e^{-x^2/\ell^2}}{\sqrt{\pi}\,\ell} \longrightarrow e^{-k^2\ell^2/2}$$

② → GP-gl. → $$i\hbar\frac{\partial}{\partial t}\psi(x) = \left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 + g|\psi(x,t)|^2\right]\psi(x,t)$$

$t \to \omega t = \tilde t$

$x \to x/\ell_{ho} = \tilde x$

$$i\hbar\omega\frac{\partial\tilde\psi(x)}{\partial\tilde t} = \left[\underbrace{\frac{-\hbar^2}{2m\ell_{ho}^2}}_{-\frac{\hbar\omega}{2}}\frac{\partial^2}{\partial\tilde x^2} + \frac{1}{2}\underbrace{m\omega^2\ell_{ho}^2}_{\hbar\omega}\tilde x^2 + \frac{g}{\ell_{ho}}|\tilde\psi(\tilde x,\tilde t)|^2\right]\tilde\psi(\tilde x,\tilde t)$$

a $\quad |\tilde\psi(\tilde x,\tilde t)|^2\,\tilde\psi(x,t)$

$x \to x/\ell_{ho} = \tilde{x}$

$\ell_{ho} = \sqrt{\frac{\hbar}{m\omega}}$

$-\frac{\hbar\omega}{2}$

$$i \frac{\partial \tilde\psi}{\partial \tilde t}(\tilde x) = \left[-\frac{1}{2}\frac{\partial^2}{\partial \tilde x^2} + \frac{1}{2}\tilde x^2 + \frac{g}{\ell_{ho}^D \hbar\omega} |\tilde\psi(\tilde x,\tilde t)|^2\right]\tilde\psi(x,t)$$

$\uparrow \tilde g$

$\int d\tilde x\, |\tilde\psi(x)|^2 = 1$

$x \to \tilde x = x/\ell_{ho}$

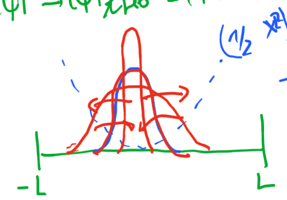
$|\tilde\psi|^2 \to |\tilde\psi|^2 \ell_{ho} = |\psi|^2$

$|\psi|^2 \sim \frac{1}{\ell_{ho}^D}|\tilde\psi|^2$

$\alpha\ a$

$$\boxed{i\frac{\partial}{\partial t}\psi(x,t) = \left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^2 + \tilde g\, |\psi(x,t)|^2\right]\psi(x,t)}$$

$\tilde g = 0$



$$\boxed{\mu\,\Phi_0(x) = \left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^2 + \tilde g\, |\Phi_0(x)|^2\right]\Phi_0(x)}$$

$\Phi_0(x)$

• Grundstand: $\psi(x,t+\Delta t) = e^{-iH\Delta t}\psi(x,t)$

Imaginäre Zeitentwicklung $\to$ $t \to -i\tau$

$$\psi(x,\tau+\Delta\tau) = e^{-H\Delta\tau}\psi(x,\tau)$$

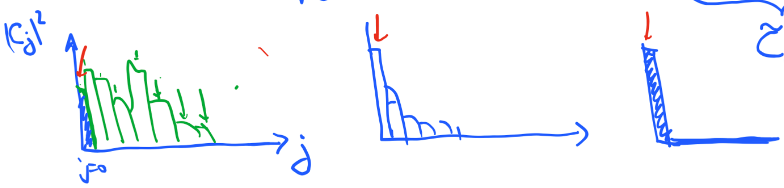
$$\psi(x,\tau) = \sum_{j=0}^{\infty} c_j(\tau)\,\phi_j(x) \quad \to \quad H\phi_j(x) = \varepsilon_j\,\phi_j(x)$$

$j=0 \to \varepsilon_0 < \varepsilon_{j\neq 0}$

$$\underbrace{e^{-H\Delta\tau}\psi(x,\tau)}= \sum_{j=0}^{\infty} c_j(\tau)\, e^{-\varepsilon_j\Delta\tau}\,\phi_j(x) = \eta(x,\tau)$$

$\int|\psi(x,\tau)|^2 = 1 \longrightarrow N = \int|\eta(x,\tau)|^2\,dx$

$$\psi(x,\tau+\Delta\tau) = \frac{1}{N}\,e^{-H\Delta\tau}\psi(x,\tau) = \sum_{j=0}^{\infty}\underbrace{\left[\frac{c_j(\tau)\,e^{-\varepsilon_j\Delta\tau}}{\sqrt N}\right]}_{c_j(\tau+\Delta\tau)}\phi_j(x)$$



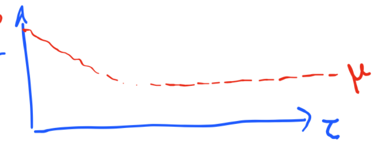
τ groß $\to$ $\psi(x,\tau) \simeq \phi_0(x)$

$$e^{-H\Delta\tau}\psi(x,\tau) \simeq e^{-\mu\Delta\tau}\phi_0(x) = \eta(x)$$

$$N = \int|\eta(x)|^2 \cong e^{-2\mu\Delta\tau}\int|\phi_0(x)|^2 dx = e^{-2\mu\Delta\tau}$$

$$N \simeq e^{-2\mu\Delta\tau} \to \ln N = -2\mu\Delta\tau \to \boxed{\mu = \frac{-\ln N}{2\Delta\tau}}$$

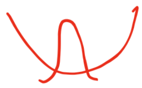
$$\boxed{-\frac{\ln N}{2\Delta\tau}}$$



1. $\Psi_0 = \psi(x, \tau=0)\ ; \quad S_0 = \text{etwas}$
2. $\tau \to \tau + \Delta\tau : \quad e^{-H\Delta\tau}\, \psi(x,\tau) = \eta(x)$
3. $N = \int |\eta(x)|^2 dx$
4. $\psi(x,\tau+\Delta\tau) = \frac{\eta(x)}{\sqrt{N}}$
5. $S = -\frac{\ln N}{2\Delta\tau} \longrightarrow \boxed{\frac{S(\tau+\Delta\tau) - S(\tau)}{S(\tau+\Delta\tau)} \overset{?}{<} \varepsilon \simeq 10^{-6}}$

NEIN: $S(\tau+\Delta\tau)$ → 2

JA: $\boxed{\begin{matrix}\psi(x,\tau+\Delta\tau) = \Phi_0(x) \\ S = \mu\end{matrix}}$

$g = 0 \longrightarrow$  $\quad V(x) = \frac{1}{2}x^2 \quad \longrightarrow \quad \frac{e^{-x^2/2}}{\sqrt{\pi}}$

- Problem mit DDWW $\Big\}$ $\int d^3r'\ V(\vec r - \vec r')\ |\psi(\vec r')|^2$

$V(\vec r) = \frac{d^2}{r^3}\left(1 - 3\cos^2\theta\right)$

$\int \frac{d^3k}{(2\pi)^3}\ \frac{4\pi}{3}\left(3\cos^2\theta - 1\right)\ \tilde n(\vec k)$

$r \to 0 \quad$ 1/0