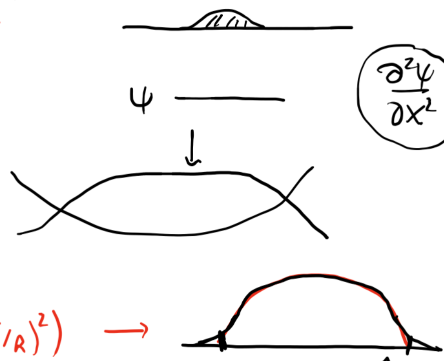
$$\mu\cancel{\psi} = \left[\cancel{H_{kin}} + V(x) + g\,n(x)\right]\cancel{\psi}$$

$g>0$



$$\frac{\partial^2\psi}{\partial x^2}$$

$$\mu = \frac{1}{2}x^2 + g\,n(x)$$

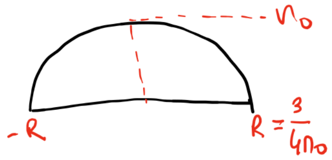
$$n(x) = \frac{\mu}{g} - \frac{1}{2g}x^2 = \frac{\mu}{g}\left[1 - \frac{1}{2\mu}x^2\right]$$

$$R^2 = 2\mu \rightarrow n(x) = n_0\left(1 - (x/R)^2\right) \rightarrow$$

$$n_0 = \mu/g \nearrow \quad 1 = \int n(x)\,dx = \int_{-R}^{R} n_0\left(1 - \left(\frac{x}{R}\right)^2\right)dx = n_0 R\int_{-1}^{1} dx\,(1-x^2) = \frac{4}{3}n_0 R = 1$$

$$\left.\begin{aligned} n_0 &= \mu/g \\ R &= \sqrt{2\mu} \end{aligned}\right\} \quad \frac{4}{3}\sqrt{2}\,\frac{1}{g}\mu^{3/2} = 1 \rightarrow \boxed{\mu = \left(\frac{3g}{4\sqrt{2}}\right)^{2/3}}$$

$$\boxed{n(x) = \frac{1}{g}\left(\frac{3g}{4\sqrt{2}}\right)^{2/3}\left[1 - \frac{x^2}{2\left(\frac{3g}{4\sqrt{2}}\right)^{2/3}}\right]}$$



Thomas-Fermi

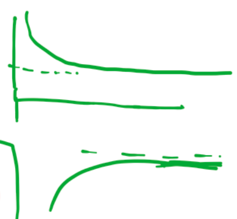
$$\boxed{\psi(t)} \xrightarrow{\Delta t} \tilde{\psi}(t+\Delta t) \longrightarrow \psi(t+\Delta t) = \frac{\tilde{\psi}(t+\Delta t)}{\sqrt{N}}$$

$$\underbrace{N = \int|\tilde{\psi}(x,t+\Delta t)|^2 dx}$$

$$\boxed{\frac{e^{-x^2/a^2}}{\sqrt{\pi}\,a}}$$

$$\psi(x) = e^{-2}$$

$n(x)$



$$\underbrace{\int dx\,|\psi_{GS}(x,t)|^2}_{N} = e^{-2\mu\Delta t}\underbrace{\int dx\,|\psi_{GS}(x)|^2}_{1} \Rightarrow N \simeq e^{-2\mu\Delta t}$$

$$\boxed{\mu = -\frac{1}{2\Delta t}\ln(norm)}$$

$$0 \longrightarrow \Delta t \longrightarrow 2\Delta t$$

$$\mu_{att} = -\frac{1}{2\Delta t}\ln(norm) \qquad \mu = -\frac{\ln(norm)}{2\Delta t}$$

$$\varphi_{rel} = \left|\frac{\mu - \mu_{att}}{\mu}\right| < \varepsilon \simeq 10^{-6} \xrightarrow{NEW} \mu_{att} = \mu$$

$>A$

STOP

$$E = \langle \psi(x) | H | \psi(x) \rangle$$
$$= \int dx\, \psi^*(x) \left[\frac{-\hbar^2}{2m} \psi(x) + V(x) + \frac{g}{2} |\psi(x)|^2 \right) \psi(x)$$

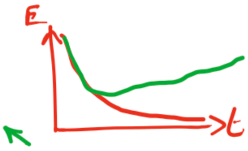
$$\int \psi^*(x) \mu \psi(x)\, dx = \int \psi^*(x) \left[-\frac{\hbar^2}{2m} \psi(x) + V(x)\psi(x) + g|\psi(x)|^2 \psi(x) \right] dx$$

$$\underbrace{\mu \int |\psi|^2 dx}_{1} = \mu = E + \frac{1}{2} g \int dx\, |\psi(x)|^4$$

$$\boxed{E = \mu - \frac{1}{2} g \underbrace{\int dx\, |\psi(x)|^4}}$$

$$\sum_j |\psi_j|^4 \Delta x$$

t	E	μ
t_0	E	



$$\mu \psi(r) = \left[-\cancel{\frac{1}{2}\nabla^2} + \frac{1}{2} r^2 + g\, n(r) \right] \psi(r)$$

T.F. $\rightarrow$ $\mu = \frac{1}{2} r^2 + g\, n(r) \rightarrow n(r) = \frac{\mu}{g} \left[1 - \frac{r^2}{2\mu} \right]$ $\quad R = \sqrt{2\mu}$

$$= \mu/g \, (1 - (r/R)^2)$$

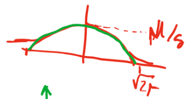
$$1 = \int n(r) d^3 r = 4\pi \int_0^{R/R} \left(\frac{r}{R}\right)^2 d\left(\frac{r}{R}\right) \frac{\mu}{g} (1 - (r/R)^2)$$

$$= \frac{\mu}{g} 4\pi R^3 \underbrace{\int_0^1 dr\, r^2 (1 - r^2)}_{2/15} = \frac{8\pi}{15} \frac{\mu R^3}{g} = \frac{8\pi}{15} \frac{2\sqrt{2}}{g} \mu^{5/2}$$

$$\mu = \left(\frac{15 g}{16 \sqrt{2} \pi} \right)^{2/5} \rightarrow n_0 = \mu/g, \quad R = \sqrt{2\mu}$$

$\boxed{V(r) = \frac{1}{2} r^2}$

$x = y = 0$



$\rightarrow$ FFT

$\boxed{\text{FFT}^{1D}}$

$$\psi(x,y,z) \rightarrow \psi(k_x, y, z) \rightarrow \psi(k_x, k_y, z) \rightarrow \psi(k_x, k_y, k_z)$$

$\boxed{\text{FFT}^{3D}}$

$$1 = \int_0^R dr\, r\, 2\pi \frac{\mu}{g} (1 - (r/R)^2)$$
$$= 2\pi \frac{\mu}{g} R^2 \int_0^1 dr\, \underbrace{r(1 - r^2)}_{1/2 - 1/4 = 1/4}$$
$$= \frac{\pi}{2} \frac{\mu}{g} 2\mu \stackrel{!}{=} 1$$
$$\mu = \sqrt{\frac{g}{\pi}}$$

FFT

- Nächste Schritte
  - ↳ Konvergenzkriterion
  - ↳ 2D, 3D Code

$\vec{k}\cdot\vec{r} = kr\cos\phi$

- $\tilde{\psi}(k) = \int dx\, \psi(x)\, e^{ikx}$

$$\tilde{\psi}(\vec{k}) = \int d^2r\, \psi(r)\, e^{i\vec{k}\vec{r}} = \int dr\, r\, \psi(r) \underbrace{\int d\phi\, e^{ikr\cos\phi}}_{2\pi J_0(kr)}$$

$$= 2\pi \int_0^\infty r\, dr\, \psi(r)\, J_0(kr) \leftarrow \mathcal{O}(N^2)$$

FFT $\mathcal{O}(N^2 \ln N)$

FFT^{2D}

$$\underbrace{\int dx \left(\underbrace{\int dy\, \psi(x,y)\, e^{ik_y y}}_{FT_y} \right) e^{ik_x x}}_{FT_x}$$

DDNW $\quad g\, n(\vec{r}) + \int d^3r'\, V(\vec{r}-\vec{r}')\, n(\vec{r}')$

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

$$\tilde{V}(\vec{k}) = \frac{4\pi}{3} d^2 (3\cos^2\theta_k - 1)$$

$$U(\vec{r}) = \int d^3r'\, V(\vec{r}-\vec{r}')\, n(\vec{r}') = \int \frac{d^3k}{(2\pi)^3}\, e^{i\vec{k}\vec{r}} \left[\tilde{V}(\vec{k})\, \tilde{n}(\vec{k}) \right]$$

k^2

$$\boxed{U(\vec{r}) = \left(\mathrm{FFT}^{-1} \left[\tilde{V}(\vec{k}) \cdot \mathrm{FFT}[n(\vec{r})](\vec{k}) \right] \right)(\vec{r})}$$

$3\frac{k_z^2}{k^2} - 1$

$k = 0$

$$e^{-i(V(\vec{r}) + g\, n(\vec{r}) + U(\vec{r}))\Delta t}\, \psi(\vec{r})$$

- $k^2 = k_x^2 + k_y^2 + k_z^2$