

Physikalische Chemie II	Matheseminar II	15.11.18
Wiederholung:		
$\hat{H}\psi_n = E_n \cdot \psi_n$ ↓ Eigenfunktion ↓ Eigenwert $\hookrightarrow E_n \in \mathbb{R}$	$\hat{H} = \text{hermitisch}$ $\int f^* \hat{H} g d\tau = \int (\hat{H} f)^* \cdot g d\tau$ $\Leftrightarrow \langle f \hat{H} g \rangle = \langle \hat{H} f g \rangle$	(müssen aber gleichwertig integrierbar sein)
$\langle \psi_n \psi_m \rangle = \delta_{n,m}$: vollständig		
$f = \sum_n c_n \cdot \psi_n$		
$\rightarrow c_n$ über Projektion $c_n = \langle \psi_n f \rangle$		
wenn f normiert wird		
$\hookrightarrow \langle f f \rangle = 1 = \sum_n c_n^* c_n = \sum_n c_n ^2 = 1 \quad c_n ^2 \geq 0 \Leftrightarrow P_n = c_n ^2$		
$\hookrightarrow \int f^* \cdot f d\tau = \int f ^2 d\tau = 1$ $ f ^2 > 0$ Wahrscheinlichkeitsdichte		
\rightarrow Wahrscheinlichkeit bestimmen: $\iiint_V \underbrace{f(x,y,z)}_{ f ^2} d\tau = P(a < x,y,z < b)$		
$\int f^* \hat{H} f d\tau = \int \left(\sum_n c_n^* \psi_n^* \right) \hat{H} \left(\sum_m c_m \psi_m \right) d\tau$		
$\langle f \hat{H} f \rangle = \sum_n \sum_m c_n^* c_m \langle \psi_n \hat{H} \psi_m \rangle$ $\hookrightarrow E_m = \langle \psi_n \hat{H} \psi_m \rangle$		
$= \sum_n \sum_m c_n^* c_m \cdot E_m \cdot \delta_{n,m}$		
$\langle f \hat{H} f \rangle = \sum_n c_n ^2 \cdot E_n = \sum_n P_n \cdot E_n = \langle E \rangle$ \rightarrow Erwartungswert		
$\langle 1 \rangle = \langle f \hat{1} f \rangle$		
falls f nicht normiert ($\langle f f \rangle \neq 1$): $\langle A \rangle = \frac{\langle f \hat{A} f \rangle}{\langle f f \rangle}$		
falls $c_n = \delta_{n,k} \rightarrow f = \psi_k \rightarrow \hat{H} \psi_k = \lambda_k \psi_k \Rightarrow \langle A \rangle = \lambda_k$		

Wiederholung:

$$\hat{H}\psi_n = E_n \cdot \psi_n$$

\downarrow Eigenfunktion \downarrow Eigenwert
 $\hookrightarrow E_n \in \mathbb{R}$

\hat{H} = hermitisch

$$\int f^* \hat{H}g d\tau = \int (\hat{H}f)^* \cdot g d\tau$$

$$\Leftrightarrow \langle f | \hat{H}g \rangle = \langle \hat{H}f | g \rangle$$

(müssen aber gut über-
integrierbar sein)

$$\langle \psi_n | \psi_m \rangle = \delta_{nm} : \text{vollständig}$$

$$f = \sum_n c_n \cdot \psi_n$$

$\rightarrow c_n$ über Projection $c_n = \langle \psi_n | f \rangle$

wenn f normiert wird

$$\hookrightarrow \underbrace{\langle f | f \rangle}_{=1} = 1 = \sum_n c_n^* c_n = \sum_n |c_n|^2 = 1 \quad |c_n|^2 \geq 0 \Rightarrow P_n = |c_n|^2$$

$$\hookrightarrow \int f^* \cdot f d\tau = \int |f|^2 d\tau = 1$$

Wahrscheinlichkeits-
dichte

\rightarrow Wahrscheinlichkeit bestimmen $\iiint_V \underbrace{|f(x,y,z)|^2}_{|f|^2} d\tau = P(a \leq x,y,z, \leq b)$

$$\int \int f^* \hat{H} f d\tau = \int \left(\sum_n c_n^* \psi_n^* \right) \hat{H} \left(\sum_m c_m \psi_m \right) d\tau$$

$$\langle f | \hat{H} f \rangle = \sum_n \sum_m c_n^* c_m \langle \psi_n | \hat{H} \psi_m \rangle$$

$\hookrightarrow = E_m \cdot \psi_m$

$$= \sum_n \sum_m c_n^* c_m \cdot E_m \cdot \delta_{nm}$$

$$\langle f | \hat{H} f \rangle = \sum_n |c_n|^2 \cdot E_n = \sum_n P_n \cdot E_n = \langle E \rangle \quad \rightarrow \text{Erwartungswert}$$

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

falls f nicht normiert ($\langle f | f \rangle \neq 1$): $\langle A \rangle = \frac{\langle f | \hat{A} f \rangle}{\langle f | f \rangle}$

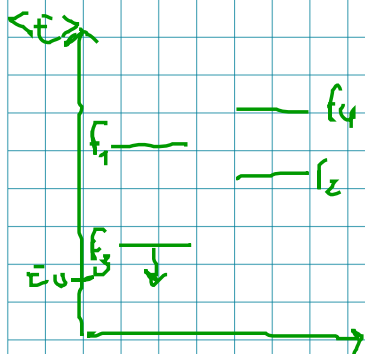
Falls $c_k = \delta_{nk} \Rightarrow f = \psi_k \Rightarrow \hat{A} f_k = \lambda_k f_k \Rightarrow \langle A \rangle = \lambda_k$

Es soll gelten $E_0 < E_1 < E_2 < \dots$

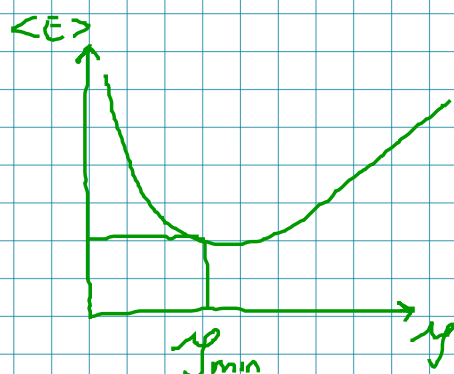
$$\langle E \rangle = \sum_n |C_n|^2 E_n = |C_0|^2 \cdot E_0 + \sum_{n=1}^{\infty} |C_n|^2 E_n$$

$$\sum_{n=0}^{\infty} |C_n|^2 = 1 \rightarrow |C_0|^2 = 1 - \sum_{n=1}^{\infty} |C_n|^2$$

$$\begin{aligned} \langle E \rangle &= \left(1 - \sum_{n=1}^{\infty} |C_n|^2\right) \cdot E_0 + \sum_{n=1}^{\infty} |C_n|^2 E_n \\ &= E_0 + \sum_{n=1}^{\infty} |C_n|^2 (E_n - E_0) \geq E_0 \rightarrow \text{Grundzustandsenergie} \end{aligned}$$



$$f(\gamma) \rightarrow \langle A \rangle(\gamma) = \langle f | \hat{A} | f \rangle$$



$$\frac{d\langle E \rangle(\gamma)}{d\gamma} = 0$$

$$\rightarrow \langle E \rangle(\gamma_{\min}) \geq E_0$$

Variationsverfahren

$$f = \sum_n C_n \varphi_n \rightarrow \langle E \rangle = \langle \sum_n C_n \varphi_n | \hat{H} | \sum_m C_m \varphi_m \rangle$$

$$= \sum_n \sum_m C_n^* C_m \underbrace{\langle \varphi_m | \hat{H} | \varphi_n \rangle}_{H_{mn}}$$

$$= \sum_n \sum_m C_n^* C_m H_{nm}$$

$$\hat{H} = \begin{pmatrix} H_{11} & H_{12} & \dots & H_{110} \\ \vdots & \vdots & \ddots & \vdots \\ H_{101} & \dots & \dots & H_{1010} \end{pmatrix} \quad H_{nm} = H_{mn}^* \quad ; \quad \text{hermitesche Matrix}$$

$$\frac{\partial \langle E \rangle}{\partial C_n} = 0 \rightarrow 10 \times 10 \text{ lineares GS, homogen} \quad \text{Ritzsches Variationsverfahren}$$

$$\hat{A}\hat{B} \neq \hat{B}\hat{A} \Rightarrow [\hat{A}, \hat{B}]_- = \hat{A}\hat{B} - \hat{B}\hat{A}$$

$$[\hat{A}, \hat{B}]_- \hat{f} = 0 \rightarrow \hat{A}\hat{f} = \lambda \hat{f}$$

$$\hat{B}\hat{f} = \mu \hat{f}$$

$$\langle \hat{A}\hat{B}\psi | \psi \rangle - \langle \psi | \hat{A}\hat{B}\psi \rangle = \langle A \rangle$$

$$[\hat{A}, \hat{B}]_- \neq 0$$

$$\Delta\hat{A} = \hat{A} - \langle A \rangle \quad \Delta\hat{B} = \hat{B} - \langle B \rangle$$

$$\delta b_A^2 = \langle \Delta A^2 \rangle = \langle \psi | \Delta\hat{A}^2 \psi \rangle = \langle \Delta\hat{A}\psi | \Delta\hat{A}\psi \rangle = \|\langle \Delta\hat{A}\psi \rangle\|^2$$

$$\delta b_B^2 = \|\langle \Delta\hat{B}\psi \rangle\|^2$$

$$\delta b_A^2 - \delta b_B^2 = \|\langle \Delta\hat{A}\psi \rangle\|^2 \cdot \|\langle \Delta\hat{B}\psi \rangle\|^2 \geq \|\langle \Delta\hat{A}\psi | \Delta\hat{B}\psi \rangle\|^2 = \|\underbrace{\langle \psi | \Delta\hat{A} \Delta\hat{B} \psi \rangle}_{*}\|^2$$

Cauchy - Schwarz - Ungleichung

$$\langle f | f \rangle \cdot \langle g | g \rangle \geq |\langle f | g \rangle|^2 \Rightarrow \|f\|^2 \cdot \|g\|^2 \geq |\langle f | g \rangle|^2$$

$$* (\hat{A} - \langle A \rangle)(\hat{B} - \langle B \rangle) = \hat{A}\hat{B} - \hat{A}\langle B \rangle - \langle A \rangle\hat{B} + \langle A \rangle\langle B \rangle$$

$$\langle \Delta\hat{A}\psi | \Delta\hat{B}\psi \rangle = \langle \psi | \hat{A}\hat{B}\psi \rangle - \langle B \rangle \underbrace{\langle \psi | \hat{A}\psi \rangle}_{\langle A \rangle} - \langle A \rangle \underbrace{\langle \psi | \hat{B}\psi \rangle}_{\langle B \rangle} +$$

$$\langle A \rangle \langle B \rangle \underbrace{\langle \psi | \psi \rangle}_{1}$$

$$= \langle \psi | \hat{A}\hat{B}\psi \rangle - \langle A \rangle \langle B \rangle$$

$$\langle \Delta\hat{B}\psi | \Delta\hat{A}\psi \rangle$$

$$= \langle \psi | \hat{B}\hat{A}\psi \rangle - \langle B \rangle \langle A \rangle$$

} voneinander abziehen

$$\langle \Delta\hat{A}\psi | \Delta\hat{B}\psi \rangle - \langle \Delta\hat{B}\psi | \Delta\hat{A}\psi \rangle = \langle \psi | [\hat{A}, \hat{B}]_- \psi \rangle = 2i \operatorname{Im}(\langle \Delta\hat{A}\psi | \Delta\hat{B}\psi \rangle)$$

$$\Downarrow$$

$$\langle \Delta\hat{A}\psi | \Delta\hat{B}\psi \rangle$$

$$\langle f | g \rangle = \int f^* g d\tau$$

$$\langle g | f \rangle = \int g^* f d\tau$$

$$= \left(\int g \cdot f^* d\tau \right)^*$$

$$= \langle f | g \rangle^*$$

$$z = a + ib$$

$$z^* = a - ib$$

$$z - z^* = 2ib$$

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

$$\langle \hat{A} \hat{B} \psi | \hat{B} \hat{A} \psi \rangle^2 = \text{Re}^2(\langle \hat{A} \hat{B} \psi | \hat{A} \hat{B} \psi \rangle) + \text{Im}^2(\langle \hat{A} \hat{B} \psi | \hat{A} \hat{B} \psi \rangle)$$

$$\Delta A \Delta B \geq \text{Im}(\langle \hat{A} \hat{B} \psi | \hat{A} \hat{B} \psi \rangle)$$

$$= \left(\frac{\langle \psi | [\hat{A}, \hat{B}] \psi \rangle}{2i} \right)^2$$

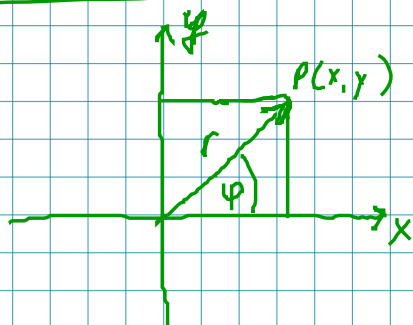
$$\Delta A \cdot \Delta B \geq \frac{1}{2i} |\langle \psi | [\hat{A}, \hat{B}] \psi \rangle| \Rightarrow \Delta x \Delta p \geq \frac{1}{2i} i\hbar = \frac{\hbar}{2}$$

$$\hat{A} = x \quad \hat{B} = -i\hbar \frac{d}{dx}$$

$$[\hat{A}, \hat{B}] = \left[x, -i\hbar \frac{d}{dx} \right] = -i\hbar \left(x \frac{d}{dx} - \frac{d}{dx} x \right)$$

$$= -i\hbar$$

Polarkoordinaten



$$x = r \cdot \cos \varphi$$

$$y = r \cdot \sin \varphi$$

$$r = \sqrt{x^2 + y^2}$$

$$\varphi = \arctan\left(\frac{y}{x}\right)$$

$$f(x, y) = f(x[r, \varphi], y[r, \varphi]) = f(r, \varphi)$$

$$\text{Vorteil} = \tilde{f}(r, \varphi) = \tilde{f}_r(r) \cdot \tilde{f}_\varphi(\varphi)$$

$$\tilde{f}(r, \varphi) = \tilde{f}(r)$$

$$df = \left(\frac{\partial f}{\partial x}\right)_y dx + \left(\frac{\partial f}{\partial y}\right)_x dy \quad dx = \left(\frac{\partial x}{\partial r}\right)_\varphi dr + \left(\frac{\partial x}{\partial \varphi}\right)_r d\varphi$$

$$= f_x (\cos \varphi dr - r \sin \varphi d\varphi) + f_y (\sin \varphi dr + r \cos \varphi d\varphi)$$

$$dx = \cos \varphi dr - (r \cdot \sin \varphi) d\varphi$$

$$dy = \sin \varphi dr + r \cdot \cos \varphi d\varphi$$

$$= \underbrace{(\cos \varphi f_x + \sin \varphi f_y)}_{\frac{\partial f}{\partial r}} dr$$

$$+ \underbrace{(-r \sin \varphi f_x + r \cdot \cos \varphi f_y)}_{\frac{\partial f}{\partial \varphi}} d\varphi = d\tilde{f}$$

$$\tilde{f}(r, \varphi) = \tilde{f}(r) \quad \frac{\partial \tilde{f}}{\partial r} = \frac{d\tilde{f}}{dr} = (f_x, f_y) \begin{pmatrix} \cos \varphi \\ \sin \varphi \end{pmatrix}$$

$$\text{Nabla-Operator: } \vec{\nabla} = \begin{pmatrix} \partial/\partial x \\ \partial/\partial y \end{pmatrix}$$

$$\Delta = \vec{\nabla} \cdot \vec{\nabla} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$$

Laplace-Operator.

Physikalische Chemie II

Matheseminar

16.11.2018

Wiederholung:

Polarkoordinaten

$$(x, y) \rightarrow (r, \varphi)$$

$$x = r \cdot \cos \varphi \quad y = r \sin \varphi$$

$$r = \sqrt{x^2 + y^2} \quad \varphi = \arctan\left(\frac{y}{x}\right)$$

$$-\infty < x, y < \infty$$

$$0 \leq \varphi \leq 2\pi$$

$$0 \leq r < \infty$$

$$f(x, y) \rightarrow \tilde{f}(r, \varphi)$$

$$df = d\tilde{f}$$

$$df = f_x dx + f_y dy$$

$$dx = \cos \varphi dr - (-1 \sin \varphi) d\varphi$$

$$d\tilde{f} = f_r dr + f_\varphi d\varphi$$

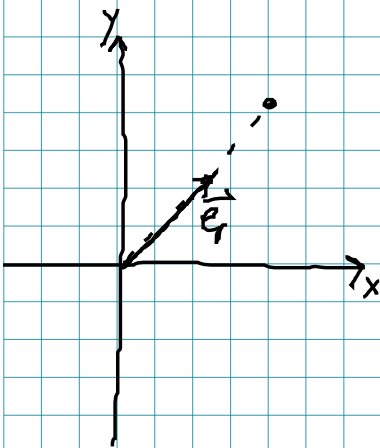
$$dr = \frac{x}{\sqrt{x^2+y^2}} dx + \frac{y}{\sqrt{x^2+y^2}} dy$$

$$\vec{\nabla} = \begin{pmatrix} \partial/\partial x \\ \partial/\partial y \end{pmatrix}$$

$$\Delta = \vec{\nabla}^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$$

$$\tilde{f}(r, \varphi) = \tilde{f}(r)$$

$$\vec{\nabla} \tilde{f} = \begin{pmatrix} \frac{\partial \tilde{f}}{\partial x} \\ \frac{\partial \tilde{f}}{\partial y} \end{pmatrix} = \begin{pmatrix} \frac{d\tilde{f}}{dr} \cdot \frac{x}{r} \\ \frac{d\tilde{f}}{dr} \cdot \frac{y}{r} \end{pmatrix} = \frac{1}{r} \cdot \frac{d\tilde{f}}{dr} \cdot \begin{pmatrix} x \\ y \end{pmatrix} = \frac{d\tilde{f}}{dr} \cdot \underbrace{\begin{pmatrix} x \\ y \end{pmatrix}}_{\vec{e}_r}$$



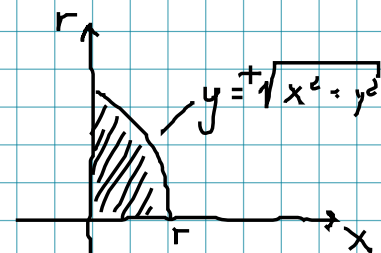
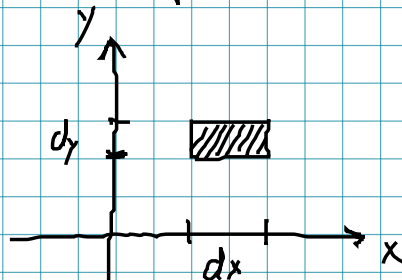
$$\frac{\partial}{\partial x} = \frac{d\tilde{f}}{dr} \cdot \frac{\partial r}{\partial x} + \frac{d\tilde{f}}{d\varphi} \cdot \frac{\partial \varphi}{\partial x}$$

$$\frac{\partial}{\partial y} = \frac{d\tilde{f}}{dr} \cdot \frac{\partial r}{\partial y} + \frac{d\tilde{f}}{d\varphi} \cdot \frac{\partial \varphi}{\partial y}$$

$$\frac{\partial^2}{\partial x^2} = \left(\frac{\partial r}{\partial x} \cdot \frac{\partial}{\partial r} + \frac{\partial \varphi}{\partial x} \cdot \frac{\partial}{\partial \varphi} \right) \cdot \left(\frac{\partial r}{\partial x} \cdot \frac{\partial}{\partial r} + \frac{\partial \varphi}{\partial x} \cdot \frac{\partial}{\partial \varphi} \right)$$

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y) dx dy$$

Flächenelement

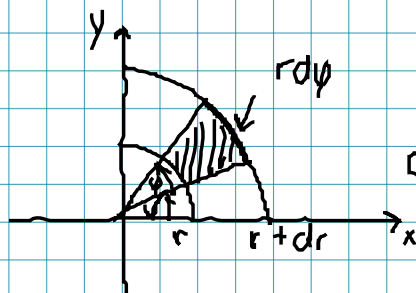


$$f(x, y) = f_r(x) = f_c(y)$$

$$(1) f \rightarrow \tilde{f}(r, \varphi)$$

(2) Grenzen $x, y \rightarrow$ Grenzen von r, φ

$$(3) dx dy \rightarrow dr d\varphi$$



$$d\tilde{V} = r dr d\varphi$$

(Metrik)

$$\int_0^{2\pi} \int_0^{\infty} \tilde{f}(r, \varphi) \cdot r \, dr \, d\varphi$$

$$(1) \tilde{f}(r, \varphi) = R(r) \cdot \Phi(\varphi)$$

$$\rightarrow \left(\int_0^{\infty} r \cdot R(r) \, dr \right) \cdot \left(\int_0^{2\pi} \Phi(\varphi) \, d\varphi \right)$$

$$(2) \tilde{f}(r, \varphi) = R(r)$$

$$\Phi(\varphi) = 1$$

$$\int_0^{2\pi} 1 \, d\varphi = 2\pi$$

$$R(r) = 1 \quad \int_0^{R_0} 2\pi r \, dr = \pi R_0^2 \quad R(r) = \delta(r - r_0) \quad \text{Deltafunktion}$$

$$R(r) = \delta(r - r_0) \quad \int_0^{\infty} 2\pi r \cdot \delta(r - r_0) \, dr = 2\pi r_0 \int_{-\infty}^{\infty} \delta(r_0 - r) \cdot f(r) \, dr = f(r_0)$$

$$\int_{-\infty}^{\infty} e^{-x^2} \, dx \quad I_x = I_y = \int_{-\infty}^{\infty} e^{-y^2} \, dy = \sqrt{\pi}$$

$$I^2 = I_x I_y = \left(\int_{-\infty}^{\infty} e^{-x^2} \, dx \right) \left(\int_{-\infty}^{\infty} e^{-y^2} \, dy \right) = \iint_{-\infty}^{\infty} e^{-x^2 - y^2} \, dx \, dy = \int_0^{2\pi} \int_0^{\infty} e^{-r^2} r \, dr \, d\varphi$$

$$= 2\pi \cdot \int_0^{\infty} r e^{-r^2} \, dr = 2\pi \left[-\frac{1}{2} e^{-r^2} \right]_0^{\infty} = \pi$$

$$\left. \begin{aligned} dx &= \left(\frac{\partial x}{\partial r} \right) dr + \left(\frac{\partial x}{\partial \varphi} \right) d\varphi \\ dy &= \left(\frac{\partial y}{\partial r} \right) dr + \left(\frac{\partial y}{\partial \varphi} \right) d\varphi \end{aligned} \right\} \begin{pmatrix} dx \\ dy \end{pmatrix} = \begin{pmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \varphi} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \varphi} \end{pmatrix} \cdot \begin{pmatrix} dr \\ d\varphi \end{pmatrix}$$

$$d\vec{r} = \hat{j} \cdot d\vec{q}$$

$$\underbrace{\begin{pmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \varphi} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \varphi} \end{pmatrix}}_{\text{Jacobian matrix} = \hat{j}}$$

$$\hat{j}^{-1} d\vec{r} = \underbrace{\hat{j}^{-1} \cdot \hat{j}}_{\hat{e}} d\vec{q} = d\vec{q}$$

$$\begin{pmatrix} dx & 0 \\ 0 & dy \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} dx \\ dy \end{pmatrix} = d\vec{r}$$

$$\hat{A} \cdot \vec{e} = d\vec{r}$$

$$\begin{pmatrix} dr & 0 \\ 0 & d\varphi \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} dr \\ d\varphi \end{pmatrix}$$

$$\hat{Q} \cdot \vec{e} = d\vec{q}$$

$$\hat{A} \cdot \vec{e} = \hat{j} \cdot \hat{Q} \cdot \vec{e}$$

$$|\hat{A}| \cdot |\vec{e}| = |\hat{j}| \cdot |\hat{Q}| \cdot |\vec{e}|$$

$$\left. \begin{array}{l} |\hat{A}| = dx dy \\ |\hat{Q}| = dr d\varphi \end{array} \right\} dx dy = |\hat{j}| \cdot dr d\varphi$$

$$\downarrow \quad \downarrow$$

$$\quad \quad \quad \text{Jacobian-} \quad \quad \quad dx dy = r dr d\varphi$$

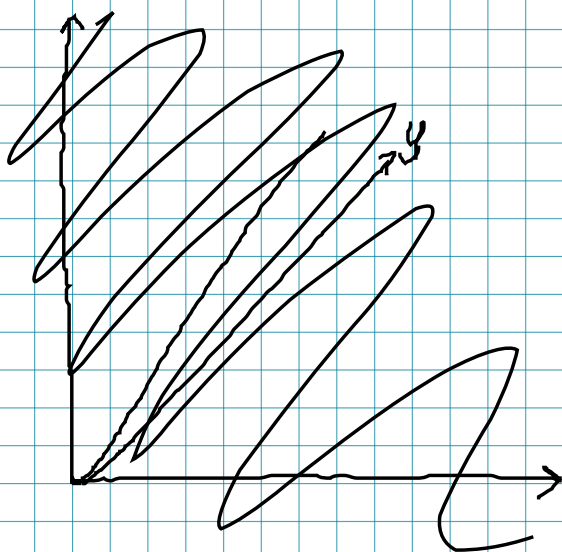
$$\quad \quad \quad \text{Determinante}$$

$$|\hat{j}| = \begin{vmatrix} \cos \varphi & -r \sin \varphi \\ \sin \varphi & r \cos \varphi \end{vmatrix} = r \cos^2 \varphi + r \sin^2 \varphi = r$$

Kugelkoordinaten

$$(x, y, z) \longrightarrow (r, \varphi, \vartheta)$$

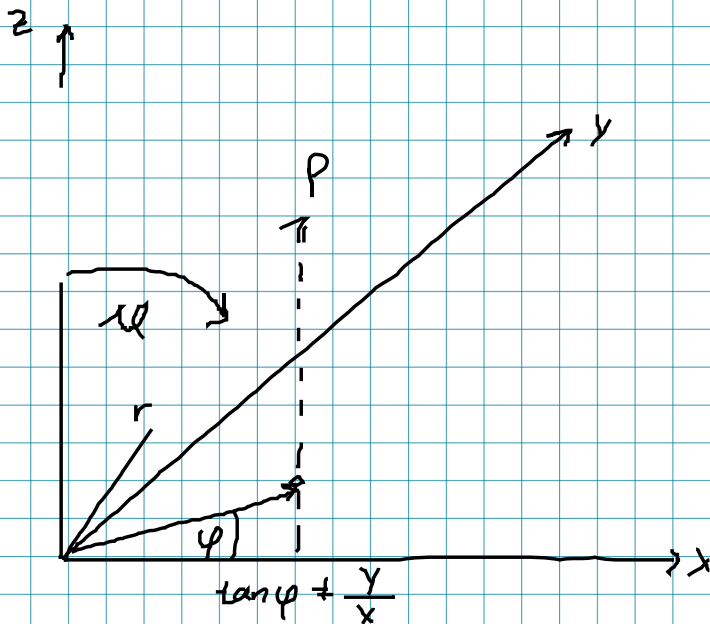
$$r = \sqrt{x^2 + y^2 + z^2}$$



ϑ = Breitengrad

$$0 \leq \vartheta \leq \pi$$

$$0 \leq \varphi \leq 2\pi$$



$$x = r \cdot \sin \vartheta \cdot \cos \varphi$$

$$y = r \cdot \sin \vartheta \cdot \sin \varphi$$

$$z = r \cdot \cos \vartheta$$

$$x^2 + y^2 = r^2 \sin^2 \vartheta$$

$$z^2 = r^2 \cos^2 \vartheta$$

$$\tan^2 \vartheta = \frac{x^2 + y^2}{z^2}$$

$$\tan \vartheta = \sqrt{\frac{x^2 + y^2}{z^2}}$$

$$(x, y, z) = \vec{f}(r, \vartheta, \varphi) \quad \begin{array}{l} \text{Kugelflächenfunktion} \\ \text{Kugelkoordinaten} \end{array}$$

$$= R(r) \cdot \gamma(\vartheta, \varphi)$$

$$\downarrow$$

$$\Phi(\varphi) \cdot \Theta(\cos \vartheta)$$

$$\left(\frac{\partial x}{\partial r}\right) = \sin \vartheta \cos \varphi \quad \left(\frac{\partial x}{\partial \vartheta}\right) = r \cdot \cos \vartheta \cos \varphi \quad \left(\frac{\partial x}{\partial \varphi}\right) = -r \cdot \sin \vartheta \cdot \sin \varphi$$

$$\left(\frac{\partial y}{\partial r}\right) = \sin \vartheta \sin \varphi \quad \left(\frac{\partial y}{\partial \vartheta}\right) = r \cos \vartheta \cdot \sin \varphi \quad \left(\frac{\partial y}{\partial \varphi}\right) = r \sin \vartheta \cos \varphi$$

$$\left(\frac{\partial z}{\partial r}\right) = \cos \vartheta \quad \left(\frac{\partial z}{\partial \vartheta}\right) = -r \sin \vartheta \quad \left(\frac{\partial z}{\partial \varphi}\right) = 0$$

$$dx dy dz = |\hat{J}| dr d\vartheta d\varphi = r^2 \sin \vartheta dr d\vartheta d\varphi$$

$$\iiint_{-\infty}^{\infty} f(x, y, z) dx dy dz = \int_0^{\infty} \int_0^{\pi} \int_0^{2\pi} \tilde{f}(r, \vartheta, \varphi) r^2 \cdot \sin \vartheta dr d\vartheta d\varphi \quad \tilde{f} = R(r)$$

$$= \left(\int_0^{\infty} r^2 \cdot R(r) dr \right) \cdot \left(\int_0^{\pi} \sin \vartheta d\vartheta \right) \cdot \left(\int_0^{2\pi} d\varphi \right)$$

$$\text{Raumwinkel } 4\pi: = 2\pi \cdot \left[-\cos \vartheta \right]_0^{\pi} \cdot \int_0^{\infty} r^2 \cdot R(r) dr = 4\pi \int_0^{\infty} r^2 R(r) dr$$

$$f_x(u_x) = N \cdot e^{-\frac{m u_x^2}{2k_B T}}$$

$$\int_{-\infty}^{\infty} f(u_x) dx = 1$$

$$f(u_x, u_y, u_z) = f_x \cdot f_y \cdot f_z$$

$$\iiint_{-\infty}^{\infty} f(u_x, u_y, u_z) du_x du_y du_z = 1$$

$$u = \sqrt{u_x^2 + u_y^2 + u_z^2}$$

$$\rightarrow g(u, \vartheta, \varphi) = N^3 e^{-\frac{m \cdot u^2}{2k_B T}} \iiint_{0}^{2\pi} \int_{0}^{\pi} \int_{0}^{\infty} g(u, \vartheta, \varphi) u^2 \cdot \sin \vartheta du d\vartheta d\varphi$$

$$N^3 \iiint_{0}^{2\pi} \int_{0}^{\pi} \int_{0}^{\infty} e^{-\frac{m u^2}{2k_B T}} \cdot u^2 du d\vartheta d\varphi \sin \vartheta = 4\pi N^3 \int_{0}^{\infty} u^2 \cdot e^{-\frac{m u^2}{2k_B T}} du$$

$$f(u) = 4\pi u^2 N^3 \cdot e^{-\frac{m u^2}{2k_B T}} \left. \vphantom{f(u)} \right\} \text{ radiale Dichte} = 1$$