e) Darstellung von Operatoren

(i) $$\boxed{A = \sum_{nm} A_{nm} |\varphi_n\rangle\langle\varphi_m| \quad \text{mit } A_{nm} = \langle\varphi_n|A|\varphi_m\rangle} \qquad (3.45)$$

... Matrix!!

(ii) $A|\psi\rangle = |\chi\rangle$

$$\rightarrow \quad \boxed{\sum_m A_{nm}\, c_m = b_n} \qquad (3.46)$$

$c_m = \langle\varphi_m|\psi\rangle \qquad b_n = \langle\varphi_n|\chi\rangle$

... Matrizenrechnung!!

(iii) $$\boxed{(AB)_{nm} = \sum_i A_{ni} B_{im}} \qquad (3.47)$$

... Matrixmultiplikation

$1 = \sum_i |\varphi_i\rangle\langle\varphi_i|$

• kontinuierliche Basis: VONS $\{\ldots|\varphi_\lambda\rangle\ldots\}$ mit $1 = \int d\lambda\, |\varphi_\lambda\rangle\langle\varphi_\lambda|$ (3.28)

analog:

$$A = \iint d\lambda\, d\lambda'\, A(\lambda,\lambda')\, |\varphi_\lambda\rangle\langle\varphi_{\lambda'}| \quad \text{mit } A(\lambda,\lambda') = \langle\varphi_\lambda|A|\varphi_{\lambda'}\rangle \qquad (3.48)$$

$$A|\psi\rangle = |\chi\rangle \longrightarrow \int A(\lambda,\lambda')\, \underbrace{c(\lambda')}_{\langle\varphi_{\lambda'}|\psi\rangle} = \underbrace{b(\lambda)}_{\langle\varphi_\lambda|\chi\rangle} \qquad (3.49)$$

$$(AB)(\lambda,\lambda') = \int d\lambda''\, A(\lambda,\lambda'')\, B(\lambda'',\lambda') \qquad (3.50)$$

• Bsp: (i) Eins-Operator 1

(3.51) $1_{nm} = \langle\varphi_n|1|\varphi_m\rangle = \delta_{nm}$ ... Diagonalmatrix

$1(\lambda,\lambda') = \langle\varphi_\lambda|1|\varphi_{\lambda'}\rangle = \delta(\lambda-\lambda')$

$$\longrightarrow 1 = \begin{cases} \sum_n |\varphi_n\rangle\langle\varphi_n| \\ \int d\lambda\, |\varphi_\lambda\rangle\langle\varphi_\lambda| \end{cases} \qquad (3.28)$$

(ii) Hamilton-Operator H:

(1) VONS $\{\dots |\varphi_n\rangle \dots\}$ $\quad n = 1, 2, \dots$

$$\left.\begin{aligned} &H_{nm} = \langle\varphi_n|H|\varphi_m\rangle \quad , \quad \langle\varphi_n|\psi\rangle = c_n \\ &\longrightarrow \langle\varphi_n|H\psi\rangle = \sum_m H_{nm} c_m \end{aligned}\right\} (9.52)$$

$$1 = \sum_m |\varphi_m\rangle\langle\varphi_m|$$

(2) Ortsdarstellung:

$$\left.\begin{aligned} &\langle \underline{r}|\hat{\underline{r}}|\underline{r}'\rangle = \underline{r}'\langle\underline{r}|\underline{r}'\rangle = \underline{r}'\,\delta(\underline{r}-\underline{r}') \\ &\langle \underline{r}|\hat{\underline{p}}|\underline{r}'\rangle = \frac{\hbar}{i}\underline{\nabla}_{\underline{r}}\,\delta(\underline{r}-\underline{r}') \end{aligned}\right\} (9.53)$$

damit:

$$\left.\begin{aligned} \langle\underline{r}|H|\underline{r}'\rangle &= \langle\underline{r}|\frac{\hat{\underline{p}}^2}{2m} + V(\hat{\underline{r}})|\underline{r}'\rangle \\ &= \left[-\frac{\hbar^2}{2m}\underline{\nabla}_r^2 + V(\underline{r}')\right]\delta(\underline{r}-\underline{r}') \\ \langle\underline{r}|H\psi\rangle &= \int d^3r'\,\langle\underline{r}|H|\underline{r}'\rangle\,\psi(\underline{r}') \\ 1 = \int d^3r'\,|\underline{r}'\rangle\langle\underline{r}'| \quad &= \left[-\frac{\hbar^2}{2m}\underline{\nabla}_r^2 + V(\underline{r})\right]\psi(\underline{r}) \end{aligned}\right\} (9.54)$$

(3) Impulsdarstellung:

$$\left.\begin{aligned} &\langle\underline{p}|\hat{\underline{p}}|\underline{p}'\rangle = \underline{p}'\langle\underline{p}|\underline{p}'\rangle = \underline{p}'\,\delta(\underline{p}-\underline{p}') \\ &\langle\underline{p}|\hat{\underline{r}}|\underline{p}'\rangle \underset{(4.40)}{=} i\hbar\underline{\nabla}_{\underline{p}}\,\delta(\underline{p}-\underline{p}') \end{aligned}\right\} (9.55)$$

damit:

$$\left.\begin{aligned} (I)\ \langle\underline{p}|H|\underline{p}'\rangle &= \langle\underline{p}|\frac{\hat{\underline{p}}^2}{2m} + V(\hat{\underline{r}})|\underline{p}'\rangle \\ &= \left[\frac{\underline{p}^2}{2m} + V(i\hbar\underline{\nabla}_{\underline{p}})\right]\delta(\underline{p}-\underline{p}') \\ \langle\underline{p}|H\psi\rangle &= \int d^3p'\,\langle\underline{p}|H|\underline{p}'\rangle\,\overline{\psi}(\underline{p}') \\ \left(1 = \int d^3p'\,|\underline{p}'\rangle\langle\underline{p}'|\right) &= \left[\frac{\underline{p}^2}{2m} + \underbrace{V(i\hbar\underline{\nabla}_{\underline{p}})}_{\text{„Differentialoperator"}}\right]\overline{\psi}(\underline{p}) \end{aligned}\right\} (9.56)$$

(II) mit $\langle \underline{p}| \underbrace{V(\hat{\underline{r}})}_{1} |\underline{p}'\rangle = \iint d^3r\, d^3r'\, \langle \underline{p}|\underline{r}\rangle\langle \underline{r}|V(\hat{\underline{r}})|\underline{r}'\rangle\langle \underline{r}'|\underline{p}'\rangle$

$$= \iint \frac{d^3r\,d^3r'}{(2\pi\hbar)^3}\, V(\underline{r})\,\delta(\underline{r}-\underline{r}')\; e^{\frac{i}{\hbar}(\underline{p}'\cdot\underline{r}'-\underline{p}\cdot\underline{r})}$$

$$= \int \frac{d^3r}{(2\pi\hbar)^3}\, V(\underline{r})\; e^{-\frac{i}{\hbar}(\underline{p}-\underline{p}')\cdot\underline{r}}$$

$$= \bar{V}(\underline{p}-\underline{p}')$$

$$\left.\begin{aligned} \longrightarrow \quad \langle \underline{p}|H|\underline{p}'\rangle &= \frac{\underline{p}^2}{2m}\,\delta(\underline{p}-\underline{p}') + \bar{V}(\underline{p}-\underline{p}') \\ \langle \underline{p}|H|\Psi\rangle &= \frac{\underline{p}^2}{2m}\,\bar{\Psi}(\underline{p}) + \underbrace{\int d^3p'\,\bar{V}(\underline{p}-\underline{p}')\,\bar{\Psi}(\underline{p}')}_{\substack{\text{Integraloperator} \\ \text{„Faltung"}}} \end{aligned}\right\} \quad (9.57)$$

- EW-Problem: $A|a_i\rangle = a_i|a_i\rangle$ (9.58) ... ~~kompakte~~ Schreibweise

Darstellung in $\{\ldots|\varphi_n\rangle\ldots\}$: $\langle\varphi_n|$(9.58) & $\mathbb{1}$ einschieben

$$\boxed{\sum_m A_{nm}\,c_m^{(i)} = a_i\,c_n^{(i)} \quad , \quad c_n^{(i)} = \langle\varphi_n|a_i\rangle} \quad (9.59)$$

.. EW-Problem in Matrizen-Form! (9.60)

kont. Basis: $\boxed{\int d\lambda'\, A(\lambda,\lambda')\,c^{(i)}(\lambda') = a_i\,c^{(i)}(\lambda) \quad , \quad c^{(i)}(\lambda) = \langle\varphi_\lambda|a_i\rangle}$

- Spektraldarstellung von A: nimm VONS der EV $\{\ldots|a_n\rangle\ldots\}$

$$A_{nm} = \langle a_n|A|a_m\rangle = a_m\,\underbrace{\langle a_n|a_m\rangle}_{\delta_{nm}}$$

$$\longrightarrow \quad \boxed{\begin{aligned} A_{nm} &= a_n\,\delta_{nm} \\ A &\underset{(9.45)}{=} \sum_n a_n |a_n\rangle\langle a_n| \end{aligned}} \quad (9.61)$$

(vgl. Matrizen/Tensoren)

analog: $A\,|a(\lambda)\rangle = a(\lambda)\,|a(\lambda)\rangle$

$$\rightarrow \boxed{\begin{aligned} A(\lambda,\lambda') &= a(\lambda)\,\delta(\lambda-\lambda') \\ A &= \int d\lambda\, a(\lambda)\, |a(\lambda)\rangle\langle a(\lambda)| \end{aligned}} \quad (3.62)$$

• Bsp:

(i) adjungierter Operator A^+

$$(A^+)_{nm} = \langle \varphi_n | A^+ | \varphi_m \rangle = \langle A\varphi_n | \varphi_m \rangle = \langle \varphi_m | A\varphi_n \rangle^*$$

$$\rightarrow \boxed{(A^+)_{nm} = A^*_{mn}} \quad (3.63)$$

[vgl. transponierte Matrix: $(T^t)_{ij} = T_{ji}$]

(ii) hermitesche Operatoren: $A = A^+$

$$\xrightarrow{(3.63)} \boxed{A_{nm} = A^*_{mn}} \quad (3.64)$$

[vgl. symmetr. Matrizen: $T_{ij} = T_{ji}$]

EW-Problem: $\rightarrow$ reelle EW, VONS von EV

(iii) unitäre Operatoren: $U^{-1} = U^+$

$$\boxed{(U^{-1})_{nm} = U^*_{mn} = (U^+)_{nm}} \quad (3.65)$$

[vgl. $\underline{\underline{D}} \in O(3)$: $(D^{-1})_{ij} = D_{ji}$]

EW-Problem $\rightarrow$ VONS von EV

f) Transformationstheorie:

• Motivation: Transformiere Darstellung bzgl. $\{\ldots|\varphi_m\rangle\ldots\}$ nach $\{\ldots|\varphi'_n\rangle\ldots\}$

$$|\varphi'_n\rangle = \mathbb{1}\,|\varphi'_n\rangle = \sum_m |\varphi_m\rangle\langle\varphi_m|\varphi'_n\rangle$$

$$\longrightarrow \boxed{|\varphi'_n\rangle = \sum |\varphi_m\rangle U_{mn} \quad \text{mit } U_{mn} = \langle\varphi_m|\varphi'_n\rangle} \quad (3.66)$$

Es gilt:

$$\boxed{\begin{aligned} &\underline{\underline{U}}\,\underline{\underline{U}}^+ = \underline{\underline{U}}^+\underline{\underline{U}} = \mathbb{1} \longleftrightarrow \underline{\underline{U}}^+ = \underline{\underline{U}}^{-1} \\ &\sum_n U_{mn}(U^+)_{nl} \overset{(3.63)}{=} \sum_n U_{mn} U^*_{ln} = \delta_{ml} \end{aligned}} \quad (3.67)$$

$\underline{\underline{U}}$ ... unitäre Matrix
vermittelt unitäre Trafo

Beweis: $\sum_n U_{mn} U^*_{ln} = \sum_n \langle\varphi_m|\varphi'_n\rangle\langle\varphi_l|\varphi'_n\rangle^*$

$$= \sum_{\underline{n}} \langle\varphi_m|\underbrace{\varphi'_n\rangle\langle\varphi'_n}_{=1}|\varphi_l\rangle = \langle\varphi_m|\varphi_l\rangle = \delta_{ml} \quad \text{qed.}$$

• Trafo zwischen Darstellungen von $|\psi\rangle$:

$$\boxed{\left.\begin{aligned} c'_n &= \langle\varphi'_n|\psi\rangle \\ c_m &= \langle\varphi_m|\psi\rangle \end{aligned}\right\} \longrightarrow \left\{\begin{aligned} c'_n &\overset{(i)}{=} \sum_m c_m U^*_{mn} = \sum_m (U^+)_{nm} c_m \\ c_m &\overset{(ii)}{=} \sum_n U_{mn} c'_n \end{aligned}\right.} \quad (3.68)$$

<u>Beweise</u>:

(i) $\langle\varphi'_n|\psi\rangle = \sum_m \underbrace{\langle\varphi'_n|\varphi_m\rangle}_{\langle\varphi_m|\varphi'_n\rangle^* = U^*_{mn}} \underbrace{\langle\varphi_m|\psi\rangle}_{c_m}$

(ii) $c_m = \sum_n U_{mn} c'_n$

setze c'_n ein

....

• Trafo zwischen Darstellungen von A:

$$\boxed{\left.\begin{aligned} A'_{nm} &= \langle\varphi'_n|A|\varphi'_m\rangle \\ A_{kl} &= \langle\varphi_k|A|\varphi_l\rangle \end{aligned}\right\} \longrightarrow \left\{\begin{aligned} A'_{nm} &\overset{(i)}{=} \sum_{ij} A_{ij} U^*_{in} U_{jm} = \sum_{ij} (U^+)_{ni} A_{ij} U_{jm} \\ A_{ij} &\overset{\text{o.B.}}{=} \sum_{nm} U_{in} A'_{nm} (U^+)_{mj} \end{aligned}\right.}$$

Beweis zu (i): $\langle\varphi'_n|\underset{1}{}A\underset{1}{}|\varphi'_m\rangle = \sum_{ij} \underbrace{\langle\varphi'_n|\varphi_i\rangle}_{U^*_{in}} \underbrace{\langle\varphi_i|A|\varphi_j\rangle}_{A_{ij}} \underbrace{\langle\varphi_j|\varphi'_m\rangle}_{U_{jm}}$ qed

- analog: (i) für kontinuierliche Basis
  (ii) für Wechsel zwischen kont. und diskreten Basis

- konkreter Fall: „$\underline{1}$ einschieben“

- Bsp: Wechsel von Orts- und Impulsdarstellung:

$$U(\underline{r},\underline{p}) = \langle \underline{r} | \underline{p} \rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{\frac{i}{\hbar} \underline{p}\cdot\underline{r}} \quad \ldots \text{ „unitäre Größe“}$$

$$\int d^3p \, U(\underline{r},\underline{p}) \, U^{+}(\underline{p},\underline{r}') = \int d^3p \, U(\underline{r},\underline{p}) \underbrace{U^{*}(\underline{r}',\underline{p})}_{\langle \underline{r}' | \underline{p} \rangle^{*}} = \underbrace{\int d^3\underline{p} \, \langle \underline{r} | \underline{p} \rangle \langle \underline{p} | \underline{r}' \rangle}_{1 \text{ (zwischen } \langle\underline{r}| \text{ und } |\underline{r}'\rangle)}$$

$$= \langle \underline{r} | \underline{r}' \rangle = \delta(\underline{r}-\underline{r}')$$