e) Darstellung von Operatoren

(i)
$$\boxed{A = \sum_{nm} A_{nm} |\varphi_n\rangle\langle\varphi_m| \quad \text{mit } A_{nm} = \langle\varphi_n|A|\varphi_m\rangle} \qquad (9.45)$$

... Matrix!!

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

$$\rightarrow \quad \boxed{\sum_m A_{nm} \underbrace{c_m}_{\langle\varphi_m|\psi\rangle} = \underbrace{b_n}_{\langle\varphi_n|\chi\rangle}} \qquad (9.46)$$

... Matrizenrechnung!!

(iii)
$$\boxed{(A\underset{\uparrow}{}B)_{nm} = \sum_i A_{ni} B_{im}} \qquad (9.47)$$

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

... Matrixmultiplikation

- kontinuierliche Basis: VONS $\{\ldots|\varphi_\lambda\rangle\ldots\}$ mit $1 = \int d\lambda\, |\varphi_\lambda\rangle\langle\varphi_\lambda|$ (9.28)

analog:

$$A = \iint d\lambda\, d\lambda'\, A(\lambda,\lambda')\, |\varphi_\lambda\rangle\langle\varphi_{\lambda'}| \quad \text{mit } A(\lambda,\lambda') = \langle\varphi_\lambda|A|\varphi_{\lambda'}\rangle \qquad (9.48)$$

$$A|\psi\rangle = |\chi\rangle \longrightarrow \int A(\lambda,\lambda')\, \underbrace{c(\lambda')}_{\langle\varphi_{\lambda'}|\psi\rangle} = \underbrace{b(\lambda)}_{\langle\varphi_\lambda|\chi\rangle} \qquad (9.49)$$

$$(AB)(\lambda,\lambda') = \int d\lambda''\, A(\lambda,\lambda'')\, B(\lambda'',\lambda') \qquad (9.50)$$

- **Bsp:** (i) Eins-Operator 1

$$(9.51) \quad \begin{aligned} 1_{nm} &= \langle\varphi_n|1|\varphi_m\rangle = \delta_{nm} \quad \text{... Diagonal-matrix} \\ 1(\lambda,\lambda') &= \langle\varphi_\lambda|1|\varphi_{\lambda'}\rangle = \delta(\lambda-\lambda') \end{aligned} \longrightarrow 1 = \begin{cases} \sum_n |\varphi_n\rangle\langle\varphi_n| \\ \int d\lambda\, |\varphi_\lambda\rangle\langle\varphi_\lambda| \end{cases} \quad (9.28)$$

(ii) Hamilton-Operator H:

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

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

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

(2) Ortsdarstellung:

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

damit:

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

$$1 = \int d^3r'\,|\underline{r}'\rangle\langle\underline{r}'|$$

(3) Impulsdarstellung:

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

damit:

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

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

$\mathbb{1}$

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

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

$$= \overline{V}(p-p')$$

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

- EW-Problem: $A|a_i\rangle = a_i |a_i\rangle$ (9.58)

  … kompakte Schreibweise

  Darstellung in $\{\dots|\varphi_n\rangle\dots\}$: $\langle\varphi_n|$(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 $\{\dots|a_n\rangle\dots\}$

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

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

(vgl. Matrizen/Tensoren)

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

$$\longrightarrow \boxed{\begin{aligned} A(\lambda,\lambda') &= a(\lambda)\,\delta(\lambda-\lambda') \\ A &= \int d\lambda\, a(\lambda)\, |a(\lambda)\rangle\langle a(\lambda)| \end{aligned}} \quad (9.62)$$

• Bsp:

(i) adjungierter Operator A^+

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

$$\longrightarrow \boxed{(A^+)_{nm} = A^*_{mn}} \quad (9.63)$$

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

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

$$\xrightarrow{(9.63)} \quad \boxed{A_{nm} = A^*_{mn}} \quad (9.64)$$

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

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

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

$$\boxed{(U^{-1})_{nm} = U^*_{mn} = (U^+)_{nm}} \quad (9.65)$$

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

EW-Problem $\longrightarrow$ VONS von EV

f) <u>Transformationstheorie</u>:

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

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

$$\rightarrow \boxed{|\varphi_n'\rangle = \sum |\varphi_m\rangle U_{mn} \quad \text{mit } U_{mn} = \langle\varphi_m|\varphi_n'\rangle} \quad (9.66)$$

Es gilt:

$$\boxed{\begin{aligned} &\underline{\underline{U}}\,\underline{\underline{U}}^+ = \underline{\underline{U}}^+\underline{\underline{U}} = \underline{\underline{1}} \longleftrightarrow \underline{\underline{U}}^+ = \underline{\underline{U}}^{-1} \\ &\sum_n U_{mn}(U^+)_{nl} \overset{(9.63)}{=} \sum_n U_{mn} U^*_{ln} = \delta_{ml} \end{aligned}} \quad (9.67)$$

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

Beweis: $\sum\limits_n U_{mn} U^*_{ln} = \sum\limits_n \langle\varphi_m|\varphi_n'\rangle\langle\varphi_l|\varphi_n'\rangle^*$

$$= \underline{\sum_n} \langle\varphi_m \underbrace{|\varphi_n'\rangle\langle\varphi_n'|}_{=1} \varphi_l\rangle = \langle\varphi_m|\varphi_l\rangle = \delta_{ml} \quad \text{qed.}$$

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

$$\boxed{\left.\begin{aligned} c_n' &= \langle\varphi_n'|\psi\rangle \\ c_m &= \langle\varphi_m|\psi\rangle \end{aligned}\right\} \longrightarrow \left\{\begin{aligned} c_n' &\overset{(i)}{=} \sum_m c_m U^*_{mn} = \sum_m (U^+)_{nm} c_m \\ c_m &\overset{(ii)}{=} \sum_n U_{mn} c_n' \end{aligned}\right.} \quad (9.68)$$

Beweise:

(i) $\langle\varphi_n'|\psi\rangle = \sum\limits_m \underbrace{\langle\varphi_n'|\varphi_m\rangle}_{\langle\varphi_m|\varphi_n'\rangle^* = U^*_{mn}} \underbrace{\langle\varphi_m|\psi\rangle}_{c_m}$

(ii) $c_m = \sum\limits_n U_{mn} c_n'$

setze c_n' ein

....

· Trafo zwischen Darstellungen von A:

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

Beweis zu (i): $\langle\varphi_n'|A|\varphi_m'\rangle = \sum\limits_{ij} \underbrace{\langle\varphi_n'|\varphi_i\rangle}_{U^*_{in}} \underbrace{\langle\varphi_i|A|\varphi_j\rangle}_{A_{ij}} \underbrace{\langle\varphi_j|\varphi_m'\rangle}_{U_{jm}}$ qed

1 1

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

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

- Bsp: Wechsel von Orts- nach Impulsdarstellung:

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

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

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